

86559

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 2/1/03
 Art Unit: 152 Phone Number 308 4519 Serial Number: 101049634
 Mail Box and Bldg/Room Location: CM 7A07 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

 Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

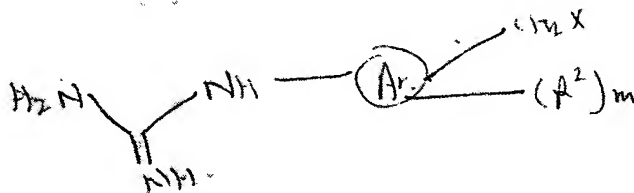
Title of Invention: Selective Inhibitors of the Urokinase Plasminogen Activator

Inventors (please provide full names): Viktor Magdolen et al.

Earliest Priority Filing Date: 8/25/99

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I

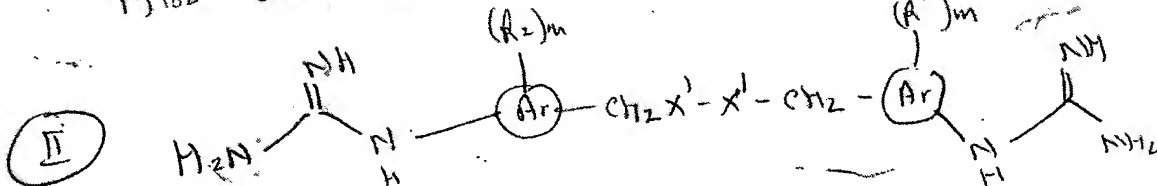


Jan Delaval
 Reference Librarian
 Biotechnology & Chemical Library
 CM1 1E07 - 703-308-4498
 jan.delaval@uspto.gov

x is NH_3R^4 , OR^3 , SR^3 , $COOR^3$, $CONR^3R^4$ for 2/18/03

See claim 15.

Also see various compounds in Table.



See claim 19

STAFF USE ONLY

Searcher: Jan

Searcher Phone #: 4458

Searcher Location: _____

Date Searcher Picked Up: 2/14/03

Date Completed: 2/16/03

Searcher Prep & Review Time: _____

Clerical Prep Time: 60

Online Time: 180

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) ✓

Bibliographic ✓

Patent Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN ✓

Dialog _____

Questel/Orbit _____

Dr.Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

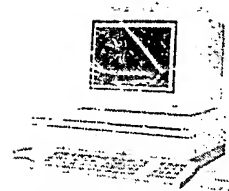
Other (specify) _____

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BioTech-Chem Library

Search Results

Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact *the BioTech-Chem searcher* who conducted the search *or contact*:

Mary Hale, Supervisor, 308-4258
CM-1 Room 1E01

Voluntary Results Feedback Form

➤ *I am an examiner in Workgroup:* (Example: 1610)

➤ *Relevant prior art **found**, search results used as follows:*

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ *Relevant prior art **not found**:*

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Search results were not useful in determining patentability or understanding the invention.

Other Comments:

Drop off completed forms at the **Circulation Desk CM-1**, or send to Mary Hale, **CM1-1E01** or e-mail **mary.hale@uspto.gov**.

Jan Delaval
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Biotechnology & Chemical Library
CM1 1E07 - 703-308-4498
jan.delaval@uspto.gov

=> d his

(FILE 'HCAPLUS' ENTERED AT 10:26:56 ON 14 FEB 2003)
DEL HIS

L1 1 S (WO2000-EP8234 OR DE99-19940389)/AP, PRN
SEL RN

FILE 'REGISTRY' ENTERED AT 10:27:43 ON 14 FEB 2003

L2 33 S E1-E33
L3 27 S L2 AND N>=3
L4 6 S L3 AND (C24H24N4O4 OR C29H32N4O6 OR C18H16F3N3O6S OR C14H22N4
L5 21 S L3 NOT L4
L6 18 S L5 AND 1/NC
L7 15 S L2 NOT L6
L8 3 S L7 AND (C19H27N5O OR C13H20N4O2 OR C16H17N5O4)
L9 21 S L6,L8

FILE 'HCAOLD' ENTERED AT 10:38:00 ON 14 FEB 2003

L10 2 S L9
SEL AN
EDIT /AN /OREF

FILE 'HCAPLUS' ENTERED AT 10:38:28 ON 14 FEB 2003

L11 4 S E34-E35
L12 3 S L11 NOT GUSEVA ?/AU

FILE 'HCAOLD' ENTERED AT 10:39:03 ON 14 FEB 2003

FILE 'HCAPLUS' ENTERED AT 10:39:14 ON 14 FEB 2003

L13 2 S L12 NOT DE947552/PN
L14 15 S L9
L15 3 S L14 AND (WILEX?/PA,CS OR (MAGDOLEN ? OR MORODER ? OR MOROEDER
L16 14 S L14 AND (PD<=20000823 OR PRD<=20000823 OR AD<=20000823)
L17 14 S L15,L16

FILE 'REGISTRY' ENTERED AT 10:50:06 ON 14 FEB 2003

L18 1 S 139639-24-0

FILE 'HCAPLUS' ENTERED AT 10:51:19 ON 14 FEB 2003

L19 6258 S L18
L20 9276 S UROKINASE(S)PLAMINOGEN(S)ACTIVAT? OR UROKINASE OR UKIDAN OR A
L21 1 S PRO() (HGF OR HEPATOCYTE GROWTH FACTOR) ()CONVERTASE
L22 5 S URINARY(S) (PLASMINOGENKINASE OR PLASMINOGEN(S)KINASE)
L23 31 S (EC OR "E C") ()3 4 21 31
L24 0 S (EC OR "E C") ()3 4 21 73
L25 12 S (EC OR "E C") ()3 4 99 26
L26 5 S L14 AND L19-L25
L27 14 S L17,L26

FILE 'USPATFULL, USPAT2' ENTERED AT 10:53:53 ON 14 FEB 2003

L28 5 S L9

=> fil reg

FILE 'REGISTRY' ENTERED AT 10:54:14 ON 14 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

DICTIONARY FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

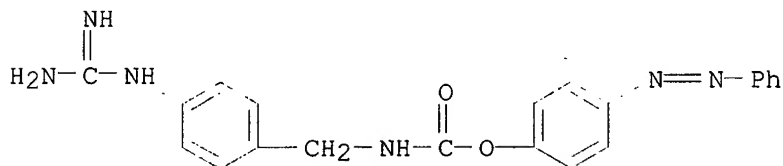
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d ide can tot 19

L9 ANSWER 1 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-77-3 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 4-(phenylazo)phenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H20 N6 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

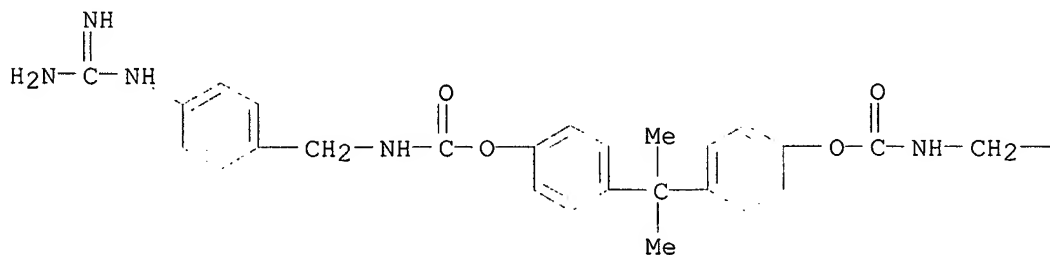


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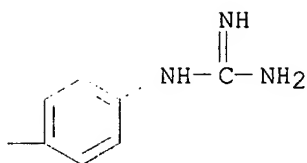
REFERENCE 1: 134:193220

L9 ANSWER 2 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-76-2 REGISTRY
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FS 3D CONCORD
MF C33 H36 N8 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PAGE 1-A

PAGE 1-B

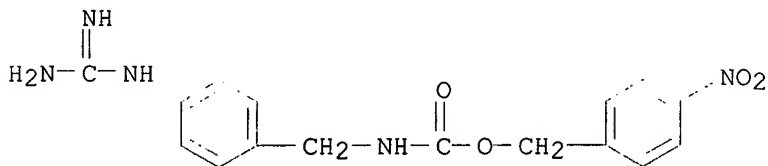


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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 3 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-75-1 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N5 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

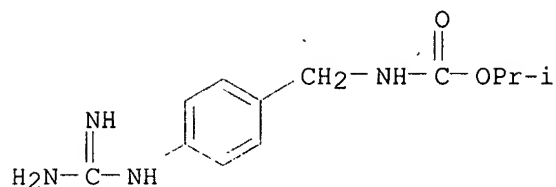


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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 4 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-74-0 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

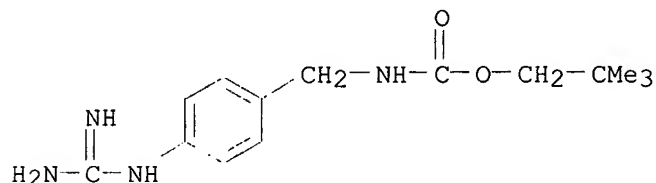


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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 5 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-73-9 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

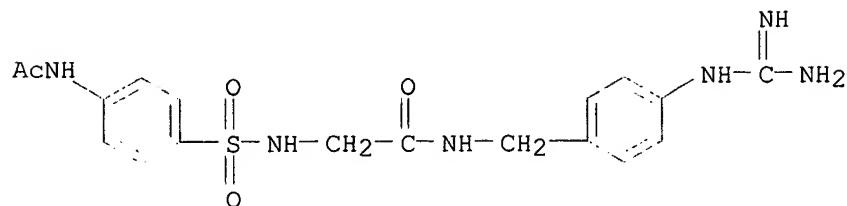


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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 6 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-72-8 REGISTRY
CN Acetamide, 2-[[[4-(acetylamino)phenyl]sulfonyl]amino]-N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

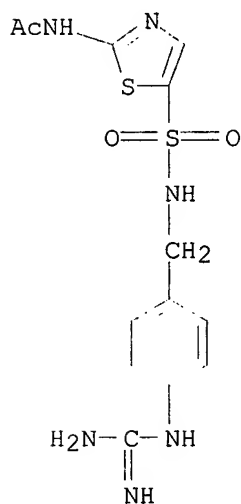


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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 7 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-71-7 REGISTRY
CN Acetamide, N-[5-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]amino]sulfonyl]-2-thiazolyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H16 N6 O3 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

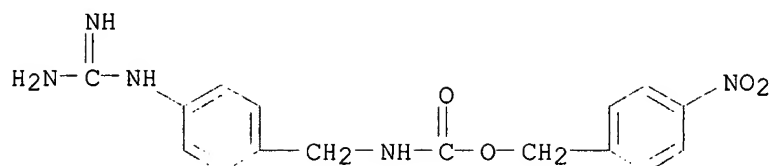


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 8 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-70-6 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, (4-nitrophenyl)methyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF C16 H17 N5 O4 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (327973-75-1)

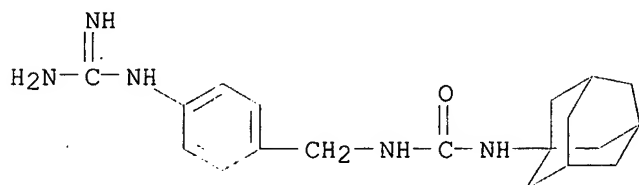


● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 9 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327973-69-3 REGISTRY
CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-tricyclo[3.3.1.1.3,7]dec-1-yl-, monohydrochloride (9CI) (CA INDEX NAME)
MF C19 H27 N5 O . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (282718-42-7)

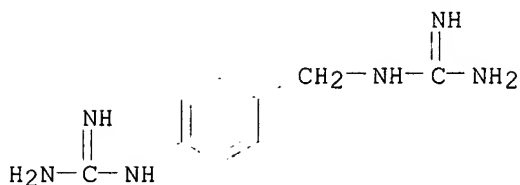


● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 10 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 327971-04-0 REGISTRY
CN Guanidine, [4-[[[(aminoiminomethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H14 N6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

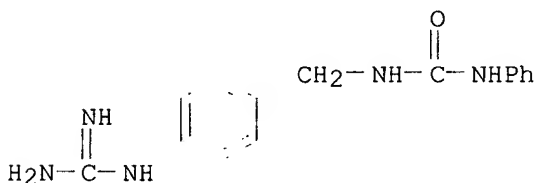


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

L9 ANSWER 11 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **282718-45-0** REGISTRY
CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C15 H17 N5 O**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



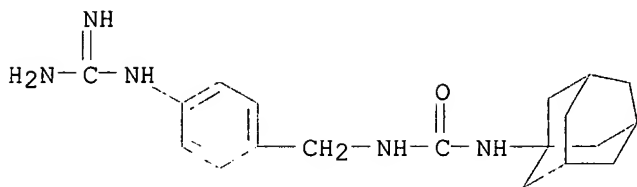
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2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 12 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **282718-42-7** REGISTRY
CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-tricyclo[3.3.1.1^{3,7}]dec-1-yl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN WX 293T
FS 3D CONCORD
MF **C19 H27 N5 O**
CI COM
SR CA
LC STN Files: CA, CAPLUS, DRUGUPDATES, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

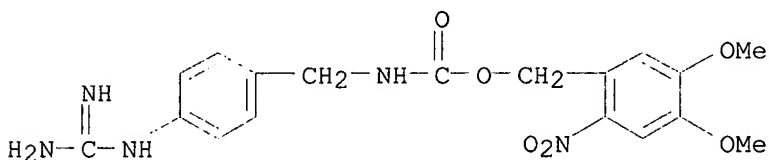
3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:276293

REFERENCE 3: 133:99075

L9 ANSWER 13 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 282718-40-5 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
(4,5-dimethoxy-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 N5 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



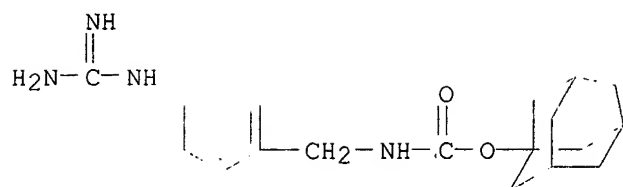
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 14 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 282718-37-0 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
tricyclo[3.3.1.1^{3,7}]dec-1-yl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H26 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



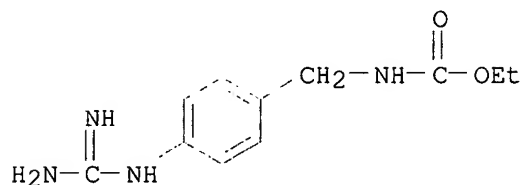
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2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 15 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 282718-36-9 REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, ethyl ester
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H16 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



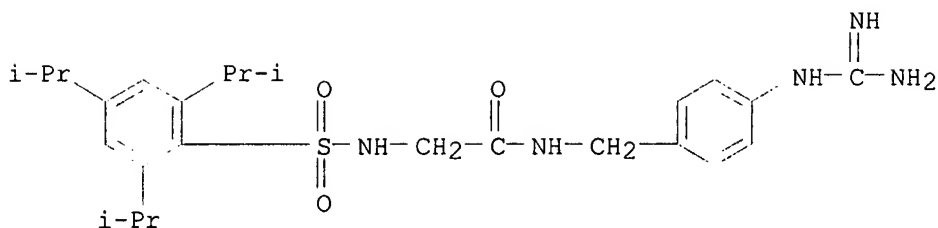
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
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REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 16 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN 282718-34-7 REGISTRY
CN Acetamide, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-2-[[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]amino]- (9CI) (CA INDEX NAME)
MF C25 H37 N5 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



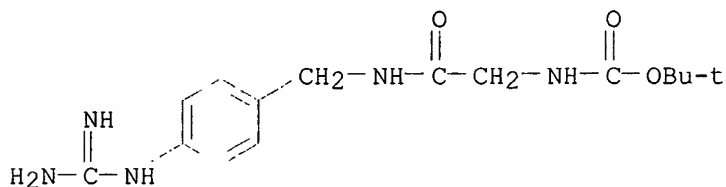
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 17 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **282718-33-6** REGISTRY
CN Carbamic acid, [2-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C15 H23 N5 O3**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



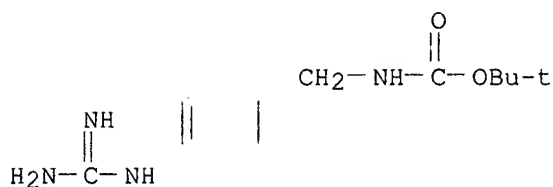
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

L9 ANSWER 18 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **202979-16-6** REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C13 H20 N4 O2**
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

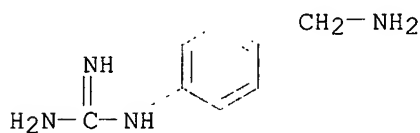
3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 133:99075

REFERENCE 3: 128:167443

L9 ANSWER 19 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **174959-56-9** REGISTRY
CN Guanidine, [4-(aminomethyl)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C8 H12 N4**
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

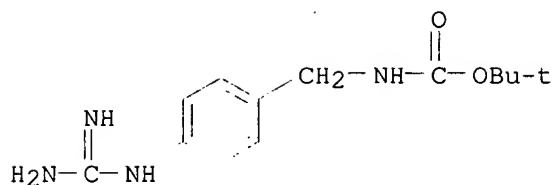
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3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:103383

REFERENCE 2: 134:193220

REFERENCE 3: 133:99075

L9 ANSWER 20 OF 21 REGISTRY COPYRIGHT 2003 ACS
RN **174959-55-8** REGISTRY
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF **C13 H20 N4 O2 . Cl H**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (202979-16-6)



● HCl

3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:193220

REFERENCE 2: 127:205895

REFERENCE 3: 124:260612

L9 ANSWER 21 OF 21 REGISTRY COPYRIGHT 2003 ACS

RN 18905-24-3 REGISTRY

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Guanidine, (p-aminophenyl)- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 4-Aminophenylguanidine

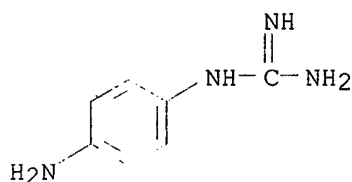
CN p-Aminophenylguanidine

FS 3D CONCORD

MF C7 H10 N4

CI COM

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
8 REFERENCES IN FILE CAPLUS (1962 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 134:193220

REFERENCE 2: 132:93320

REFERENCE 3: 128:111760

REFERENCE 4: 102:181546

REFERENCE 5: 102:108930
REFERENCE 6: 78:94208
REFERENCE 7: 58:77861
REFERENCE 8: 53:34913

=> fil hcaold
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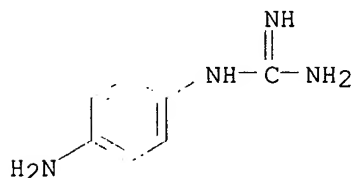
PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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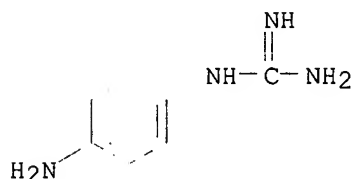
L10 ANSWER 1 OF 2 HCAOLD COPYRIGHT 2003 ACS
AN CA58:13301e CAOLD
TI ultraviolet absorption spectra, dissocn. consts., and nuclear magnetic resonance spectra of some guanidine derivs.
AU Koike, Hisashi
IT 2002-16-6 5901-56-4 14279-92-6 16060-65-4 18905-24-3
45964-97-4 54015-04-2 67453-80-9 90484-90-5
IT 18905-24-3
RN 18905-24-3 HCAOLD
CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 2 HCAOLD COPYRIGHT 2003 ACS
AN CA53:6266c CAOLD
TI 4-aminoquinaldine compds.
AU Jensch, Heinrich
PA Farbwerke Hoechst Akt.-Ges.
DT Patent
PATENT NO. KIND DATE

PI DE 950637

IT 2739-16-4 7035-79-2 7317-02-4 16060-65-4 18905-24-3
 42823-46-1 60131-35-3 98277-55-5 99178-92-4 101788-80-1 109942-84-9
 114698-68-9 115122-69-5 115122-77-5 117877-92-6 117877-93-7
 IT 18905-24-3
 RN 18905-24-3 HCAOLD
 CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 10:54:58 ON 14 FEB 2003
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FILE COVERS 1907 - 14 Feb 2003 VOL 138 ISS 8
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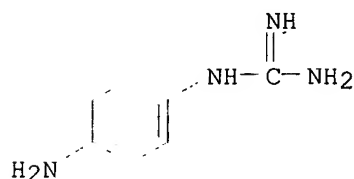
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L29 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS
 AN 1963:77861 HCAPLUS
 DN 58:77861
 OREF 58:13301e-g
 TI Ultraviolet absorption spectra, dissociation constants, and nuclear magnetic resonance spectra of some guanidine derivatives
 AU Koike, Hisashi
 CS Nagoya City Univ., Japan
 SO Nippon Kagaku Zasshi (1962), 83, 917-23
 DT Journal
 LA Unavailable
 CC 10 (Spectra and Some Other Optical Properties)
 AB Some guanidine derivs. were prepd. and their phys. properties examd. The new compd. MeCH(OH)CHNHC(:NH)NH2.HNO3 m. 114-15.degree.. pKa' of p-XC6H4NHC(:NH)NH2 (I) were obtained as follows (X and pKa' given): NO2 9.28, Cl 10.5, CO2H 10.6, H 11.0, Me 11.4, MeO 11.5, NH2 11.6, OH 12.2. The values satisfy Hammett's equation with $\rho = +2.30$. From these values, the .sigma. value of the guanidinium group can be obtained: it is +0.443

from the BzOH series, +0.377 from the PhOH series, and +0.317 from the PhNH₂ series. When CH₂O is added to guanidine derivs., pK_a' decreases by approx. 1, probably because of establishment of equil. [RNH-C-(NH₂)₂]+.dblharw. [RNH-C(NH₂)(NHCH₂OH)]+. Ultraviolet spectra of I were recorded below and above their pK_a', showing the isosbestic point. The absorption does not change much when the substituent is electron-donating, but shifts to longer wavelength in more basic media than pK_a' when the substituent is electron-withdrawing. The results suggest that the structure of phenylguanidine is shown as I. N.M.R. spectra of guanidinium salts in D₂O were also recorded. The guanidinium group has almost the same effect as OH on the .alpha.-H, but hardly affects the spectra of .beta.-H. The results were also compared with those of amines and NH₄ salts.

IT Reactions
 (consts., of guanidine derivs.)
 IT Inductive effect
 Inductive effect
 (in guanidine derivs., spectra and)
 IT Ionization
 Nuclear magnetic resonance
 Spectra, visible and ultraviolet
 (of guanidine derivs.)
 IT 2002-16-6, Guanidine, phenyl- 5901-56-4, Guanidine, (p-nitrophenyl)-
 14279-92-6, Guanidine, (p-hydroxyphenyl)- 16060-65-4, Benzoic acid,
 p-guanidino- 18905-24-3, Guanidine, (p-aminophenyl)-
 45964-97-4, Guanidine, (p-chlorophenyl)- 54015-04-2, Guanidine, p-tolyl-
 67453-80-9, Guanidine, (p-methoxyphenyl)- 90484-90-5, Guanidine,
 (2-hydroxypropyl)-, nitrate
 (ionization, nuclear magnetic resonance and spectrum of)
 IT 18905-24-3, Guanidine, (p-aminophenyl)-
 (ionization, nuclear magnetic resonance and spectrum of)
 RN 18905-24-3 HCAPLUS
 CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



=> d all hitstr 2

L29 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS
 AN 1959:34913 HCAPLUS
 DN 53:34913
 OREF 53:6266c-i,6267a
 TI 4-Aminoquinaldine compounds
 IN Jensch, Heinrich
 PA Farbwerke Hoechst Akt.-Ges. vorm. Meister Lucius & Bruning
 SO Addn. to Ger. 947,552 (preceding abstr.)
 DT Patent
 LA Unavailable
 NCL 12P; 1-10
 CC 10G (Organic Chemistry: Heterocyclic Compounds)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 950637		19561011	DE	

- AB 4-Aminoquinaldine compds. are prepd. by the following methods. (1) 4,6-Diaminoquinaldine or 6-aminoquinaldine contg. a group in the 4-position convertible to an NH₂ group is condensed with guanidinobenzoyl halides. (2) N'-(4-Amino-6-quinaldyl)diaminocyanuric chloride substituted in the 4-position by a group convertible to an NH₂ group is condensed with an aminophenylguanidine. (3) (4-Amino-6-quinaldyl azide or a 6-quinaldyl azide contg. a substituent in the 4-position convertible to an NH₂ group is condensed with a guanidinobenzyl cyanide. (4) (4-Amino-6-quinaldyl)acetonitrile or compds. substituted in 4-position by a group convertible to an NH₂ group is condensed with a guanidinophenyl azide. The substituents in the 4-position are converted to the NH₂ group after the condensation. Thus, 20 g. p-aminobenzyl cyanide-HCl, 12 g. cyanamide, and 8 cc. H₂O is heated on a water-bath, the clear melt dild. with H₂O, alkalinized with concd. NaOH, and cooled to give (p-guanidino)benzyl cyanide, m. 165-6.degree. (decompn.) (H₂O); HNO₃ salt, m. 189.degree. (decompn.). Condensing of 1 mole free base with 1 mole 2-methyl-4-amino-6-quinolyl azide in alc. soln. in the presence of 1 mole EtONa, refluxing the mixt. 1 hr., cooling, and adding a little H₂O yields 1-(2-methyl-4-amino-6-quinolyl)-4-(p-guanidinophenyl)-5-amino-1,2,3-triazole. (p-Aminophenyl)guanidine (I) carbonate (5 g.) is prepd. by reducing (p-nitrophenyl)guanidine, m. 198-9.degree. (decompn.), with H in the presence of Pd in AcOH, adding K₂CO₃ and treating I carbonate, m. 180-1.degree. (decompn.), with concd. NaOH, or by warming p-aminoacetanilide-HCl with H₂O and cyanamide, adding Na₂CO₃, recrystg. the formed (p-acetaminophenyl)guanidine carbonate from H₂O, m. 220.degree. (decompn.), and heating with dil. HCl with splitting off the Ac group. N'-(2-Methyl-4-amino-6-quinolyl)diaminocyanuric chloride (3.5 g.), and 100 g. H₂O is refluxed 3 hrs., HNO₃ added, and the nitrate of N'-(2-methyl-4-amino-6-quinolyl)-N''-(p-guanidinophenyl)melamine converted to the free base by addn. of NaOH. I carbonate (18.1 g.) is dissolved in 200 cc. H₂O and 22 cc. concd. H₂SO₄, diazotized with a soln. of 7 g. NaNO₂ in 30 cc. H₂O, a soln. of 6 g. NaN₃ in 20 cc. H₂O added with stirring and cooling, after complete reaction excess 2N HNO₃ added, and the pptd. (p-guanidinophenyl)azide nitrate (11.95 g.) recrystd. from H₂O, m. 200.degree. (decompn.); free base, recrystd. from H₂O, m. 147-8.degree. (decompn.). A soln. of 2.3 g. Na in 150 cc. EtOH and 9.85 g. (2-methyl-4-amino-6-quinolyl) acetonitrile was refluxed 1 hr., cooled, the ppt. filtered off, washed with alc. and then with warm H₂O, and recrystd. from alc. to give 1-(p-guanidinophenyl)-4-(2-methyl-4-amino-6-quinolyl)-5-(amino-1,2,3-triazole, decomp. 245.degree.. p-Aminobenzoic acid (16.2 g.), 8 cc. H₂O, and 9.7 cc. concd. HCl is mixed with 11.5 g. cyanamide, the thin paste warmed on the water-bath, the clear melt treated with sufficient amts. of dil. HCl, the soln. cooled, the thick paste of (p-guanidino)benzoic acid-HCl filtered off, and washed with dil. HCl. Addn. of Na₂CO₃ soln. yields a ppt., insol. in dil. AcOH, readily sol. in NaOH, m. 280.degree. (H₂O) with vigorous foaming. The HCl salt is converted to (p-guanidino)benzoyl chloride-HCl, by refluxing with SOCl₂ during 0.5 hr. and removing the excess SOCl₂ in vacuo. Condensation with 4,6-diaminoquinaldine in glacial AcOH, slight warming, dissolving the pptd. mass in H₂O, and pptg. with NaOH yields 2-methyl-4-amino-6-[(p-guanidino)benzoylamino]quinoline, which may be recrystd. from H₂O and alc.
- IT Acetanilide, 4'-guanidino-, carbonate
- IT Guanidine, (p-aminophenyl)-, carbonate
- IT Carbonic acid, compds. with p-[(1-acetyl-3-butenylidene)hydrazino]benzamid
ine
(with guanidine derivs.)
- IT 7035-79-2, Benzoyl chloride, p-guanidino-, hydrochloride 7317-02-4, Acetanilide, 4'-guanidino- 16060-65-4, Benzoic acid, p-guanidino- 18905-24-3, Guanidine, (p-aminophenyl)- 42823-46-1, Benzoic acid, p-guanidino-, hydrochloride 60131-35-3, Benzoyl chloride, p-guanidino- 98277-55-5, Guanidine, (p-azidophenyl)- 99178-92-4, Guanidine, (.alpha.-cyano-p-tolyl)- 109942-84-9, Guanidine, (.alpha.-cyano-p-tolyl)-, nitrate 114698-68-9, Guanidine,

(p-azidophenyl)-, nitrate 115122-69-5, Guanidine, {p-[5-amino-1-(4-amino-2-methyl-6-quinolyl)-1H-1,2,3-triazol-4-yl]phenyl}- 115122-69-5, Guanidine, {p-[5-amino-1-(4-amino-2-methyl-6-quinolyl)-1H-1,2,3-triazol-4-yl]phenyl}- 115122-77-5, Guanidine, {p-[5-amino-4-(4-amino-2-methyl-6-quinolyl)-1H-1,2,3-triazol-1-yl]phenyl}- 117877-92-6, Guanidine, {p-{{4-amino-6-[(4-amino-2-methyl-6-quinolyl)amino]-s-triazin-2-yl}amino}phenyl}- 117877-92-6, Guanidine, {p-{{4-amino-6-[(4-amino-2-methyl-6-quinolyl)amino]-s-triazin-2-yl}amino}phenyl}- 117877-93-7, Guanidine, {p-{{4-amino-6-[(4-amino-2-methyl-6-quinolyl)amino]-s-triazin-2-yl}amino}phenyl}-, nitrate

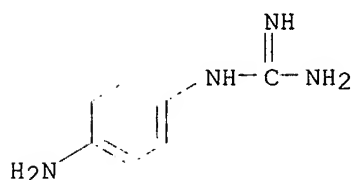
(prepn. of)

IT 18905-24-3, Guanidine, (p-aminophenyl)-

(prepn. of)

RN 18905-24-3 HCAPLUS

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



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L30 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:152638 HCAPLUS

DN 134:193220

TI Preparation of arylguanidines as selective inhibitors of urokinase plasminogen activator.

IN Magdolen, Viktor; Moroder, Luis; Sperl, Stefan
; Stuerzebecher, Joerg; Wilhelm, Olaf

PA Willex Biotechnology G.m.b.H., Germany

SO PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DT Patent

LA German

IC ICM C07C279-18

ICS A61K031-155

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001014324	A1	20010301	WO 2000-EP8234	20000823 <--
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DE 19940389	A1	20010301	DE 1999-19940389	19990825 <--
EP 1206447	A1	20020522	EP 2000-969245	20000823 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRAI DE 1999-19940389 A 19990825 <--
WO 2000-EP8234 W 20000823 <--
OS MARPAT 134:193220
AB Use of H₂N(HN:)CNHAr(CHX₁R₁)(R₂)_m [Ar = aryl, heteroaryl; X₁ = NR₃R₄, OR₃, SR₃, CO₂R₃, CONR₃R₄, COR₅; R₁ = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl, CO₂R₃, CONR₃R₄, COR₅; R₂ = halo, C(R₆)₃, C(R₆)₂C(R₆)₃, OC(R₆)₃, OC(R₆)₂C(R₆)₃; R₃ = H, org. residue; R₄ = H, (substituted) alkyl, alkenyl, alkynyl; R₅ = H, (substituted) alkyl, alkenyl, alkynyl, carboxyalkyl, carboxyalkenyl, carboxyalkynyl, carboxyaryl, carboxyheteroaryl; R₆ = H, halo (particularly F); m = 0-4], for inhibition of urokinase plasminogen activator is claimed. Thus, 4-(N-tert-butoxycarbonylaminomethyl)aniline (prepn. given) was stirred with N,N'-di-benzyloxycarbonyl-N''-trifluoromethylsulfonylguanidine in acetone to give 89% 1-[4-(tert-butoxycarbonylaminomethyl)phenyl]-2,3-di-benzyloxycarbonylguanidine. The latter was hydrogenated in MeOH over Pd/C to give 89% 4-(tert-butoxycarbonylaminomethyl)phenylguanidinium hydrochloride. This inhibited urokinase plasminogen activator with K_i = 36 .mu.M.
ST arylguanidine prepn urokinase plasminogen activator inhibitor; guanidine aryl prepn urokinase plasminogen activator inhibitor; metastasis inhibitor arylguanidine prepn; neoplasm inhibitor arylguanidine prepn
IT Antitumor agents
(metastasis; prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT Antitumor agents
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT 139639-24-0, Urokinase plasminogen activator
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(inhibitors; prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT 174959-55-8P 327973-69-3P 327973-70-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT 18905-24-3 174959-56-9 202979-16-6
282718-33-6 282718-34-7 282718-36-9
282718-37-0 282718-40-5 282718-42-7
282718-45-0 327971-04-0 327973-71-7
327973-72-8 327973-73-9 327973-74-0
327973-75-1 327973-76-2 327973-77-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT 4403-71-8, 4-Aminobenzylamine 4411-25-0, 1-Adamantyl isocyanate
4457-32-3, 4-Nitrobenzyl chloroformate 152120-54-2 207857-19-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
IT 94838-55-8P 168050-39-3P 172348-93-5P 172348-94-6P 327973-78-4P
327973-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Barber, C; WO 9920608 A 1999 HCAPLUS

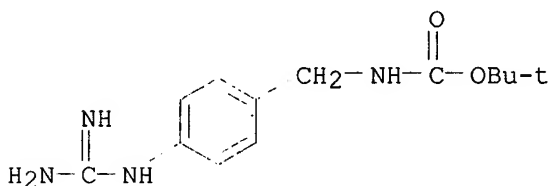
- (2) Bollag, W; Substituted Benzylhydrazines 1968, P3321 HCAPLUS
- (3) Fabrbwerke Hoechst Aktiengesellschaft; DE 947552 C 1956 HCAPLUS
- (4) Hoffmann La Roche, F, and Co, AG; CH 441366 A 1968 HCAPLUS
- (5) Patchett, A; US 3257411 A 1966 HCAPLUS
- (6) Rai, R; Journal of Medicinal Chemistry 1992, V35(22), P4150 HCAPLUS
- (7) Schacht, A; US 5914319 A 1999 HCAPLUS
- (8) Yang, H; Journal of Medicinal Chemistry 1990, V33(11), P2956 HCAPLUS

IT 174959-55-8P 327973-69-3P 327973-70-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)

RN 174959-55-8 HCAPLUS

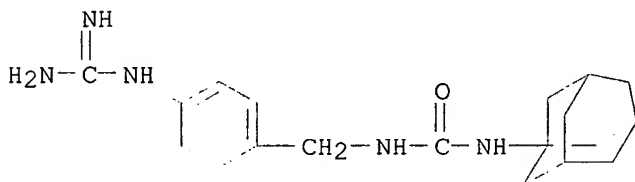
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 327973-69-3 HCAPLUS

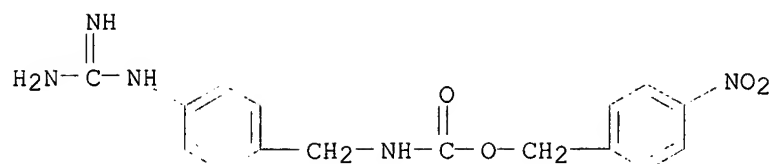
CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-tricyclo[3.3.1.1^{3,7}]dec-1-yl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 327973-70-6 HCAPLUS

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, (4-nitrophenyl)methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

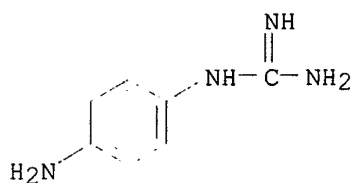
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 327973-75-1 327973-76-2 327973-77-3

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(prepn. of arylguanidines as selective inhibitors of urokinase plasminogen activator)

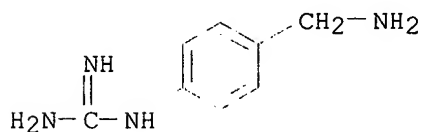
RN 18905-24-3 HCAPLUS

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



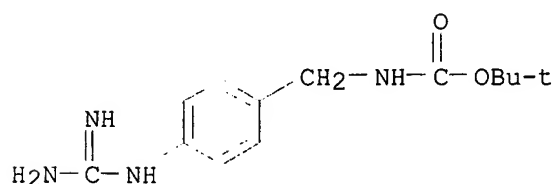
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CN Guanidine, [4-(aminomethyl)phenyl]- (9CI) (CA INDEX NAME)

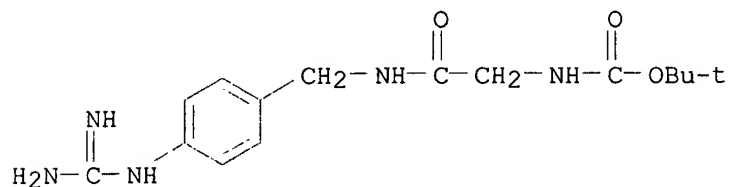


RN 202979-16-6 HCAPLUS

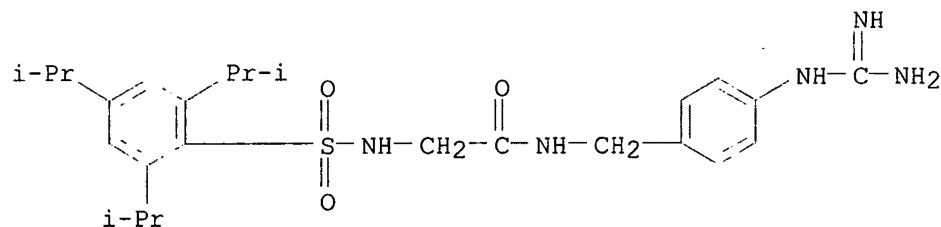
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



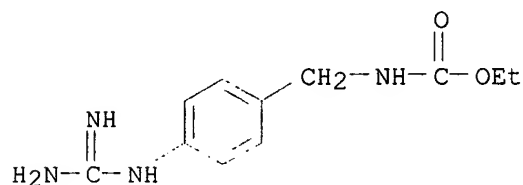
RN 282718-33-6 HCAPLUS
 CN Carbamic acid, [2-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



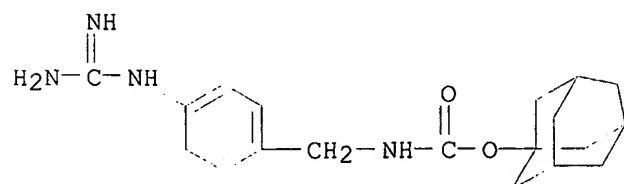
RN 282718-34-7 HCAPLUS
 CN Acetamide, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-2-[[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]amino]- (9CI) (CA INDEX NAME)



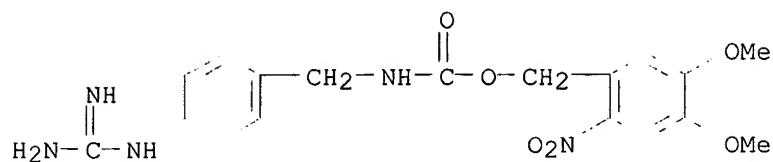
RN 282718-36-9 HCAPLUS
 CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 282718-37-0 HCAPLUS
 CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, tricyclo[3.3.1.1^{3,7}]dec-1-yl ester (9CI) (CA INDEX NAME)

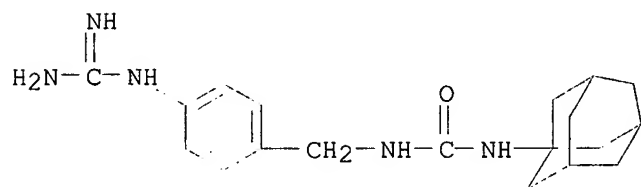


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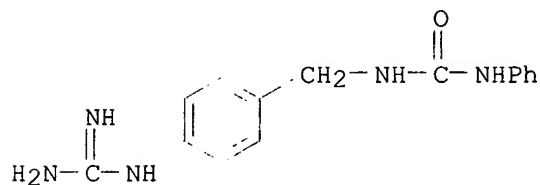
RN 282718-42-7 HCAPLUS

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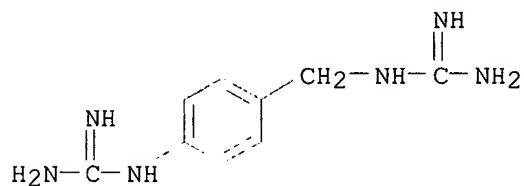
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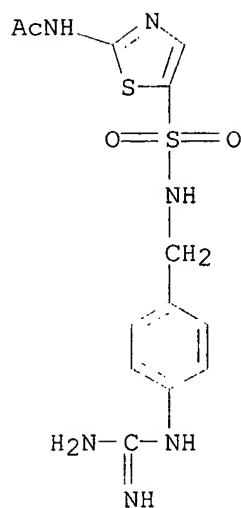
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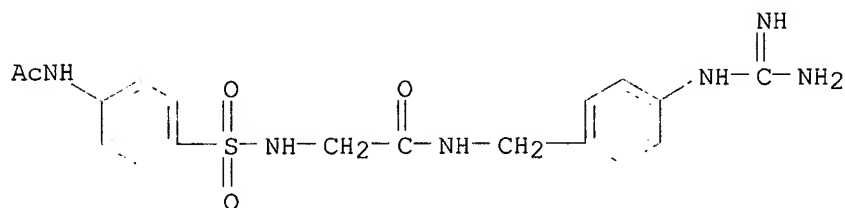
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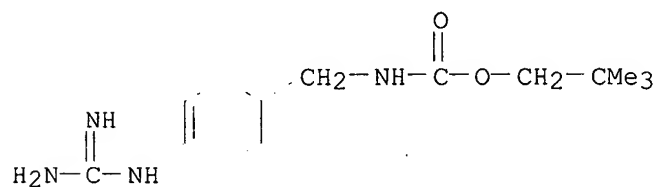
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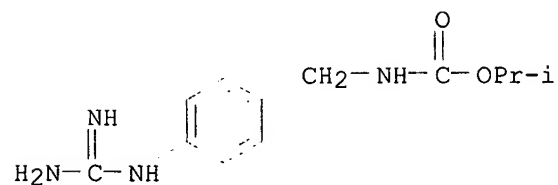
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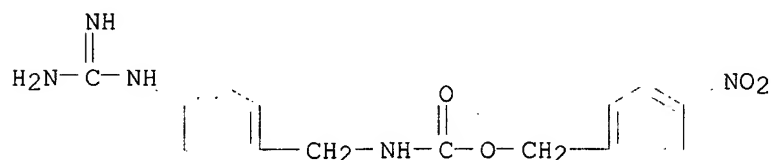


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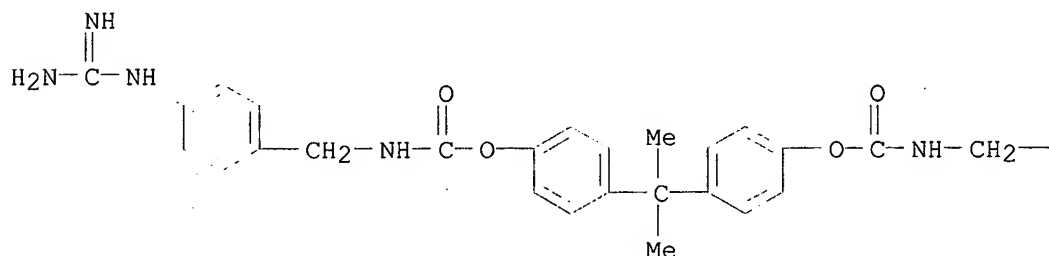
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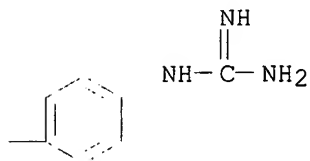
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RN 327973-76-2 HCAPLUS

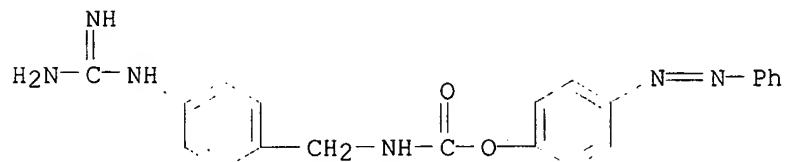
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
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PAGE 1-A

PAGE 1-B



RN 327973-77-3 HCAPLUS

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
4-(phenylazo)phenyl ester (9CI) (CA INDEX NAME)

L30 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:534024 HCAPLUS

DN 133:276293

TI Crystals of the Urokinase Type Plasminogen Activator Variant .beta.c-uPA
in Complex with Small Molecule Inhibitors Open the Way towards
Structure-based Drug Design

AU Zeslawska, Ewa; Schweinitz, Andrea; Karcher, Annette; Sondermann, Peter;

Sperl, Stefan; Sturzebecher, Jorg; Jacob, Uwe
 CS Abteilung Strukturforschung, Max-Planck-Institut fur Biochemie,
 Martinsried, D-82152, Germany
 SO Journal of Molecular Biology (2000), 301(2), 465-475
 CODEN: JMOBAK; ISSN: 0022-2836
 PB Academic Press
 DT Journal
 LA English
 CC 1-12 (Pharmacology)
 Section cross-reference(s): 7, 75
 AB Urokinase is a serine protease involved in cancer growth and metastasis.
 Here the authors present the first urokinase crystal structure in complex
 with reversible inhibitors at 2.1 and 2.6 .ANG. resolu. These inhibitor
 complex structures have been obtained from crystals of engineered
 urokinase type plasminogen activator designed to obtain a crystal form
 open for inhibitor soaking. The mutant C122S loses its flexible A-chain
 upon activation cleavage and crystallizes in the presence of benzamidine,
 which was later displaced by the desired inhibitor. This new soakable
 crystal form turned out to be of great value in the process of
 structure-based drug design. The evaluated binding mode of amiloride, and
 UKI-1D revealed a new subsite of the primary specificity pocket of
 urokinase that will be employed in the future ligand optimization process.
 (c) 2000 Academic Press.
 ST crystal structure urokinase plasminogen activator inhibitor; drug design
 urokinase plasminogen activator inhibitor
 IT Enzyme functional sites
 (active; crystals of urokinase type plasminogen activator variant
 .beta.c-uPA in complex with small mol. inhibitors open way towards
 structure-based drug design)
 IT Conformation
 Crystal structure
 Drug design
 Molecular association
 (crystals of urokinase type plasminogen activator variant .beta.c-uPA
 in complex with small mol. inhibitors open way towards structure-based
 drug design)
 IT 618-39-3, Benzamidine 2609-46-3, Amiloride 220355-63-5, UKI 1
 282718-42-7, WX 293T 300579-37-7, UKI 1D
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological
 process); BSU (Biological study, unclassified); PRP (Properties); BIOL
 (Biological study); PROC (Process)
 (crystals of urokinase type plasminogen activator variant .beta.c-uPA
 in complex with small mol. inhibitors open way towards structure-based
 drug design)
 IT 9039-53-6, Urokinase 139639-24-0, Urokinase type plasminogen activator
 RL: BPR (Biological process); BSU (Biological study, unclassified); PRP
 (Properties); BIOL (Biological study); PROC (Process)
 (crystals of urokinase type plasminogen activator variant .beta.c-uPA
 in complex with small mol. inhibitors open way towards structure-based
 drug design)

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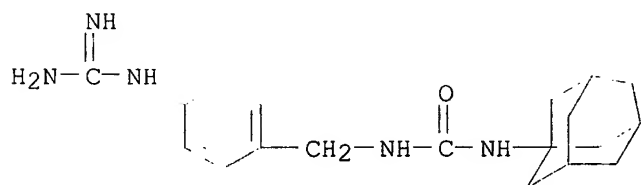
IT 282718-42-7, WX 293T

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(crystals of urokinase type plasminogen activator variant .beta.c-uPA in complex with small mol. inhibitors open way towards structure-based drug design)

RN 282718-42-7 HCAPLUS

CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-tricyclo[3.3.1.1^{3,7}]dec-1-yl- (9CI) (CA INDEX NAME)



L30 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:341443 HCAPLUS

DN 133:99075

TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective inhibitors of human urokinase

AU **Sperl, Stefan; Jacob, Uwe; De Prada, Nuria Arroyo; Sturzebecher, Jorg; Wilhelm, Olaf G.; Bode, Wolfram; Magdolen, Viktor; Huber, Robert; Moroder, Luis**

CS Max-Planck-Institut für Biochemie, Martinsried, 82152, Germany

SO Proceedings of the National Academy of Sciences of the United States of America (2000), 97(10), 5113-5118

CODEN: PNASA6; ISSN: 0027-8424

PB National Academy of Sciences

DT Journal

LA English

CC 1-3 (Pharmacology)

Section cross-reference(s): 7, 25

AB Increased expression of the serine protease urokinase-type plasminogen.

activator (uPA) in tumor tissues is highly correlated with tumor cell migration, invasion, proliferation, progression, and metastasis. Thus inhibition of uPA activity represents a promising target for antimetastatic therapy. So far, only the x-ray crystal structure of uPA inactivated by H-Glu-Gly-Arg-chloromethylketone has been reported, thus limited data are available for a rational structure-based design of uPA inhibitors. Taking into account the trypsin-like arginine specificity of uPA, (4-aminomethyl)phenylguanidine was selected as a potential P1 residue and iterative derivatization of its amino group with various hydrophobic residues, and structure-activity relationship-based optimization of the spacer in terms of hydrogen bond acceptor/donor properties led to N-(1-adamantyl)-N'-(4-guanidinobenzyl)urea as a highly selective nonpeptidic uPA inhibitor. The x-ray crystal structure of the uPA B-chain complexed with this inhibitor revealed a surprising binding mode consisting of the expected insertion of the phenylguanidine moiety into the S1 pocket, but with the adamantyl residue protruding toward the hydrophobic S1' enzyme subsite, thus exposing the ureido group to hydrogen-bonding interactions. Although in this enzyme-bound state the inhibitor is crossing the active site, interactions with the catalytic residues Ser-195 and His-57 are not obsd., but their side chains are spatially displaced for steric reasons. Compared with other trypsin-like serine proteases, the S2 and S3/S4 pockets of uPA are reduced in size because of the 99-insertion loop. Therefore, the peculiar binding mode of the new type of uPA inhibitors offers the possibility of exploiting optimized interactions at the S1'/S2' subsites to further enhance selectivity and potency. Because crystals of the uPA/benzamide complex allow inhibitor exchange by soaking procedures, the structure-based design of new generations of uPA inhibitors can rely on the assistance of x-ray anal.

ST urokinase inhibitor aminomethyl phenylguanidine structure

IT Crystal structure

Molecular association

((aminomethyl)phenylguanidine derivs. as nonpeptidic highly selective inhibitors of human urokinase)

IT Structure-activity relationship

(enzyme-inhibiting; (aminomethyl)phenylguanidine derivs. as nonpeptidic highly selective inhibitors of human urokinase)

IT 2002-16-6P 174959-56-9P 180079-82-7P 202979-16-6P

282718-30-3P 282718-31-4P 282718-32-5P 282718-33-6P

282718-34-7P 282718-35-8P 282718-36-9P

282718-37-0P 282718-38-1P 282718-39-2P 282718-40-5P

282718-41-6P 282718-42-7P 282718-43-8P 282718-44-9P

282718-45-0P 282718-46-1P 282718-47-2P 282718-48-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

((aminomethyl)phenylguanidine derivs. as nonpeptidic highly selective inhibitors of human urokinase)

IT 9001-90-5, Plasmin 9002-04-4, Thrombin 9002-05-5, Factor Xa

9002-07-7, Trypsin 139639-24-0, Urokinase-type plasminogen activator

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

((aminomethyl)phenylguanidine derivs. as nonpeptidic highly selective inhibitors of human urokinase)

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282718-34-7P 282718-36-9P 282718-37-0P

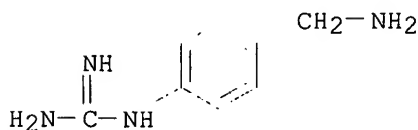
282718-40-5P 282718-42-7P 282718-45-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

((aminomethyl)phenylguanidine derivs. as nonpeptidic highly selective inhibitors of human urokinase)

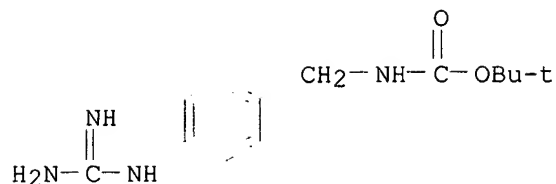
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CN Guanidine, [4-(aminomethyl)phenyl]- (9CI) (CA INDEX NAME)



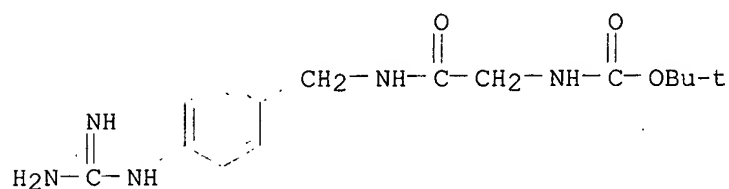
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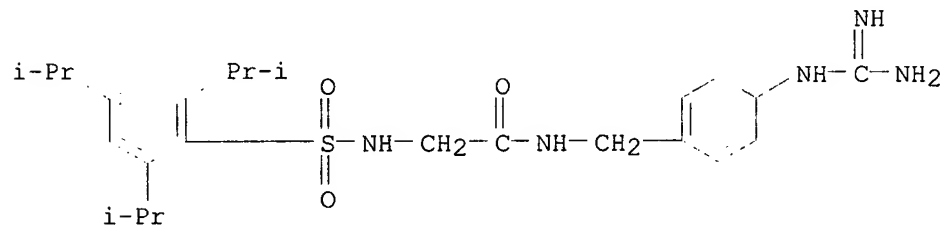
RN 282718-33-6 HCAPLUS

CN Carbamic acid, [2-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



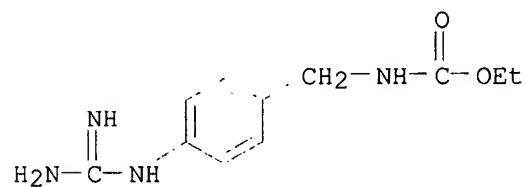
RN 282718-34-7 HCAPLUS

CN Acetamide, N-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]-2-[[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]amino]- (9CI) (CA INDEX NAME)



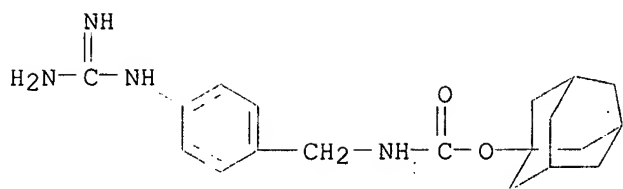
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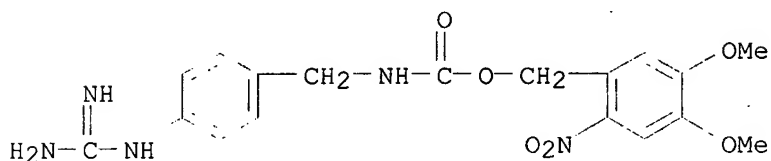


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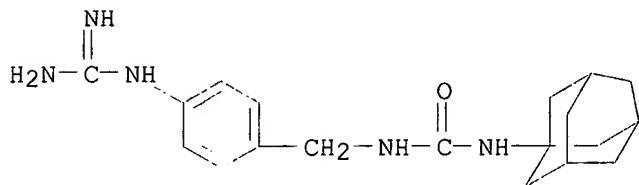
CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, tricyclo[3.3.1.1.3,7]dec-1-yl ester (9CI) (CA INDEX NAME)



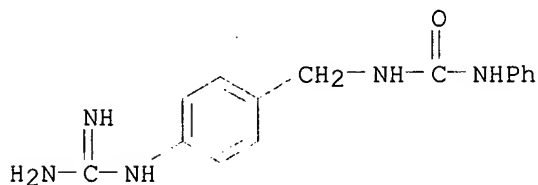
RN 282718-40-5 HCAPLUS
 CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, (4,5-dimethoxy-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



RN 282718-42-7 HCAPLUS
 CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-tricyclo[3.3.1.3^0,2^0]dec-1-yl- (9CI) (CA INDEX NAME)



RN 282718-45-0 HCAPLUS
 CN Urea, N-[[4-[(aminoiminomethyl)amino]phenyl]methyl]-N'-phenyl- (9CI) (CA INDEX NAME)



L30 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2003 ACS
 AN 2000:34861 HCAPLUS
 DN 132:93320
 TI Preparation of aminobenzimidazoles and guanidines as novel potassium channel blocking agents
 IN Teuber, Lene; Olesen, Soren-Peter; Strobaek, Dorte; Jensen, Bo Skaaning; Peters, Dan
 PA Neurosearch A/S, Den.
 SO PCT Int. Appl., 74 pp.
 CODEN: PIXXD2
 DT Patent

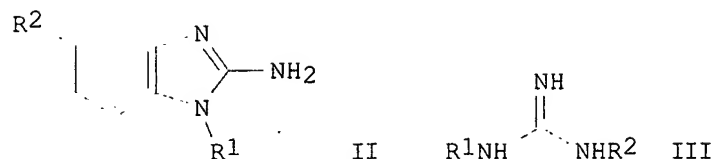
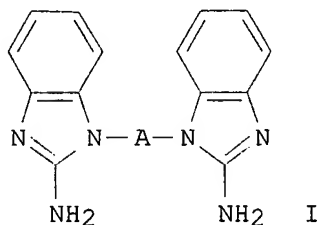
LA English
 IC ICM C07D235-30
 ICS C07D417-04; C07D403-10; C07D417-12; C07D219-08; C07D255-04;
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 A61K031-425; A61K031-435; A61K031-395; A61K031-505; A61K031-155

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000001676	A1	20000113	WO 1999-DK378	19990701 <--
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	AU 9947689	A1	20000124	AU 1999-47689	19990701 <--
	EP 1091942	A1	20010418	EP 1999-931019	19990701 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	JP 2002519412	T2	20020702	JP 2000-558081	19990701 <--
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	US 2002049246	A1	20020425	US 2000-750345	20001229 <--
	US 6380180	B2	20020430		
	US 2002137784	A1	20020926	US 2002-84179	20020228 <--
PRAI	DK 1998-865	A	19980702	<--	
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	WO 1999-DK378	W	19990701	<--	
	US 1999-347514	A3	19990702	<--	
	US 2000-750345	A3	20001229		
OS	MARPAT 132:93320				
GI					



AB The title compds. [I (A = a spacing group contg. of 1-20 atoms), II (R1 = mono- or polycyclic (un)substituted aryl, aralkyl, mono- or polycyclic heterocyclyl, etc.; R2 = H, alkyl, CF3), III (R1, R2 = H, alkyl, mono- or

polycyclic heterocyclyl, etc.), etc.], useful for the treatment or alleviation of diseases or disorders assocd. with the activity of potassium channels, in particular asthma, cystic fibrosis, chronic obstructive pulmonary disease, convulsions, vascular spasms, coronary artery spasms, renal disorders, etc., were prepd. Thus, treatment of N,N'-bis(2-aminophenyl)-1,4-butanediamine.2HCl (prepn. given) with cyanogen bromide in DMF afforded I [A = (CH)₄]. Biol. data for some of the title compds. were given.

- ST potassium channel blocker aminobenzimidazole guanidine prepn; benzimidazole prepn potassium channel blocker; antiasthmatic aminobenzimidazole guanidine prepn; cystic fibrosis aminobenzimidazole guanidine prepn; chronic obstructive pulmonary disease aminobenzimidazole guanidine prepn; lung disease chronic obstructive aminobenzimidazole guanidine prepn; anticonvulsant aminobenzimidazole guanidine prepn; vascular spasm aminobenzimidazole guanidine prepn; blood vessel spasm aminobenzimidazole guanidine prepn; renal disorder aminobenzimidazole guanidine prepn; kidney disease aminobenzimidazole guanidine prepn
- IT Lung, disease
(chronic obstructive, treatment of; prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT Ion channel blockers
(potassium; prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT Antiasthmatics
Anticonvulsants
(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT Blood vessel, disease
(spasm, treatment of; prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT Cystic fibrosis
Kidney, disease
(treatment of; prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT 158722-75-9P 188600-95-5P 254434-87-2P 254434-88-3P 254435-24-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT 5441-10-1P **18905-24-3P** 39677-07-1P 39677-08-2P 83750-38-3P
150493-50-8P 150662-77-4P 155791-73-4P 158722-44-2P 158722-55-5P
160384-00-9P 254434-69-0P 254434-70-3P 254434-71-4P 254434-72-5P
254434-73-6P 254434-74-7P 254434-75-8P 254434-76-9P 254434-77-0P
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254435-00-2P 254435-01-3P 254435-02-4P 254435-03-5P 254435-04-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)
- IT 62-53-3, Benzenamine, reactions 92-62-6, 3,6-Diaminoacridine 95-83-0, 2-Amino-4-chloroaniline 98-16-8, 3-Aminobenzotrifluoride 104-83-6, 4-Chlorobenzyl chloride 106-50-3, 1,4-Benzenediamine, reactions 109-01-3, 1-Methylpiperazine 110-60-1, 1,4-Butanediamine 110-85-0, Piperazine, reactions 110-91-8, Morpholine, reactions 121-17-5, 4-Chloro-3-nitrobenzotrifluoride 123-75-1, Pyrrolidine, reactions 504-63-2, 1,3-Propanediol 539-48-0, 1,4-Benzenedimethanamine 622-34-4, Phenylcyanamide 623-24-5 934-32-7, 2-Aminobenzimidazole 1493-27-2,

1-Fluoro-2-nitrobenzene 1664-40-0, N-Phenylethylenediamine 2010-06-2,
 2-Amino-4-phenylthiazole 3034-53-5, 2-Bromothiazole 4637-24-5
 4857-06-1, 2-Chlorobenzimidazole 6522-44-7 15801-69-1,
 4-Bromo-1,3,5-trimethylpyrazole 16825-43-7 20925-27-3,
 3-Chloro-4-cyanoaniline 30381-69-2 34403-52-6, 4-
 (Dimethylamino)benzylamine dihydrochloride 35541-78-7 42365-43-5,
 4-Chlorobenzylamine hydrochloride 43181-78-8, 1-Benzyl-2-
 chlorobenzimidazole 47375-51-9 71170-28-0 94021-22-4 150493-35-9
 158722-66-8 254435-18-2 254435-19-3 254435-20-6 254435-21-7
 254435-22-8 254435-23-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of aminobenzimidazoles and guanidines as potassium channel
 blocking agents)

IT 1619-39-2P 3840-20-8P 5418-93-9P 31067-22-8P 71173-38-1P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of aminobenzimidazoles and guanidines as potassium channel
 blocking agents)

RE.CNT 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD

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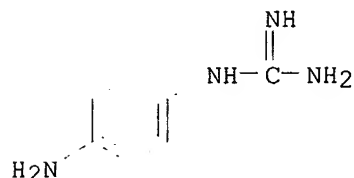
IT 18905-24-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)

RN 18905-24-3 HCAPLUS

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L30 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:102855 HCAPLUS

DN 128:167443

TI Novel compounds [cyclooctylene bis(piperazinecarboxylates) and analogs] and compositions for treating diseases associated with tryptase activity

IN Dener, Jeffrey Mark; Kuo, Elaine Yee-Lin; Rice, Ken Duane; Wang, Vivian Rueywen; Young, Wendy Beth

PA Arris Pharmaceutical Corporation, USA; Dener, Jeffrey Mark; Kuo, Elaine Yee-Lin; Rice, Ken Duane; Wang, Vivian Rueywen; Young, Wendy Beth

SO PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D295-20

ICS C07D211-26; C07D233-14; A61K031-495

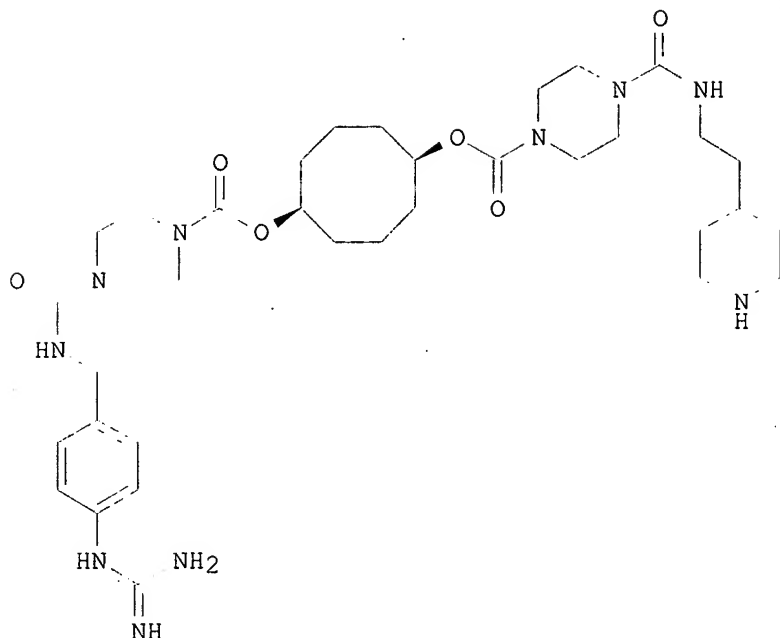
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 7

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9804537	A1	19980205	WO 1997-US13422	19970730 <--
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
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	AU 733621	B2	20010517		
	EP 934293	A1	19990811	EP 1997-937066	19970730 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
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	CN 1073103	B	20011017		
	JP 2001509787	T2	20010724	JP 1998-509136	19970730 <--
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	NO 9900433	A	19990325	NO 1999-433	19990129 <--
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LT 4587	B	19991227	LT 1999-19	19990301 <--
LV 12458	B	20000920	LV 2000-30	20000225 <--
LV 12459	B	20000920	LV 2000-31	20000225 <--
PRAI US 1996-23139P	P	19960730 <--		
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WO 1997-US13422	W	19970730 <--		
LV 1999-990027	A3	19990218 <--		
OS MARPAT 128:167443				
GI				



II

- AB The invention relates to novel compds. (R1X1X2X3X4)-X5-(X6X7X8X9R2) (I), which are tryptase inhibitors, and their pharmaceutically acceptable salts and N-oxides, as well as their uses as therapeutic agents, and methods of their prepn. [wherein X5 = (hetero)cycloalkylene, (hetero)arylene; X4, X6 = bond, alkylene; X1, X9 = bond, CO, CO2, OCO, CONR3, NR3CO, etc.; R3 = H, alkyl, cycloalkyl; X3, X7 = CO, CO2, OCO, CONR3, NR3CO, etc.; X2, X8 = (hetero)alkylene and/or cycloalkylene; R1 = amino, amidino, guanidino, certain N-heterocycles, etc., with optional (hetero)alkylene or other bridge; R2 = amino, 1-iminoethyl, methylamino, or certain N-heterocycles, with required or optional alkylene or other bridge]. The compds. are useful for treating a variety of conditions, including asthma, rheumatoid arthritis, and conjunctivitis. For instance, tert-Bu 4-[(4-guanidinobenzyl)carbamoyl]-1-piperazinecarboxylate trifluoroacetate underwent deprotection with CF3CO2H and amidation with cis-1,5-cyclooctylene chloroformate 4-(tert-butoxycarbonyl)-1-piperazinecarboxylate (77%), followed by a second deprotection and reaction with tert-Bu 4-(2-isocyanatoethyl)-1-piperidinecarboxylate, to give title compd. II. Compds. I inhibited human tryptase in vitro with IC50 in the range of 0.0001 to 41 .mu.M.
- ST cyclooctylene piperazinecarboxylate prepn tryptase inhibitor; antiasthmatic cyclooctylene piperazinecarboxylate prepn; antiarthritic cyclooctylene piperazinecarboxylate prepn; antiinflammatory cyclooctylene piperazinecarboxylate prepn
- IT Eye, disease
(conjunctivitis, treatment; prepn. of cyclooctylene

bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT Intestine, disease
 (inflammatory, treatment; prepn. of cyclooctylene
 bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT Corticosteroids, biological studies
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmaceutical compns. contg.; prepn. of cyclooctylene
 bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT Allergy inhibitors
 Anti-inflammatory agents
 Antiarthritics
 Antiasthmatics
 Antiulcer agents
 Cytotoxic agents
 (prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as
 tryptase inhibitors)
 IT Proliferation inhibition
 (proliferation inhibitors; prepn. of cyclooctylene
 bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT Skin, disease
 (treatment; prepn. of cyclooctylene bis(piperazinecarboxylates) and
 analogs as tryptase inhibitors)
 IT Adrenoceptor agonists
 (.beta.-, pharmaceutical compns. contg.; prepn. of cyclooctylene
 bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT 1822-32-8P, 4-Piperidinepropanoic acid 5462-71-5P, 4-Cyanophenylacetic
 acid 51052-79-0P 59878-28-3P 68160-42-9P 121370-60-3P
 154775-43-6P 174959-54-7P 178972-20-8P 178972-21-9P 178972-32-2P
 178972-37-7P 178972-38-8P 202979-16-6P 202979-18-8P
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 202979-30-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Préparation); RACT
 (Reactant or reagent)
 (intermediate; prepn. of cyclooctylene bis(piperazinecarboxylates) and
 analogs as tryptase inhibitors)
 IT 50-02-2, Dexamethasone 58-08-2, Caffeine, biological studies 58-55-9,
 Theophylline, biological studies 83-67-0, Theobromine 124-94-7,
 Triamcinolone 317-34-0, Aminophylline 4419-39-0, Beclomethasone
 13392-18-2, Fenoterol 16110-51-3, Cromolyn 18559-94-9, Albuterol
 23031-25-6, Terbutaline 69049-73-6, Nedocromil 73573-87-2, Formoterol
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmaceutical compns. contg.; prepn. of cyclooctylene
 bis(piperazinecarboxylates) and analogs as tryptase inhibitors)
 IT 202978-81-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
 (Reactant or reagent); USES (Uses)
 (prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as
 tryptase inhibitors)
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 202979-15-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as tryptase inhibitors)

IT 97501-93-4, Tryptase

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as tryptase inhibitors)

IT 498-94-2, Isonipecotic acid 4403-71-8, 4-Aminobenzylamine 5036-48-6, 1-(3-Aminopropyl)imidazole 23418-82-8, cis-1,5-Cyclooctanediol 27802-77-3 31166-44-6, Benzyl 1-piperazinecarboxylate 57260-71-6, tert-Butyl 1-piperazinecarboxylate 69395-13-7, 2-(4-Cyanophenyl)ethanol 98488-12-1 202979-31-5 202979-32-6 202979-33-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as tryptase inhibitors)

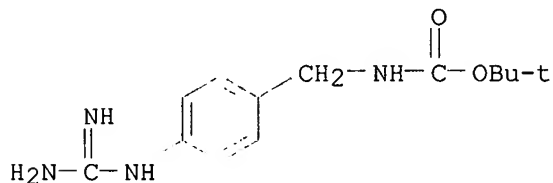
IT 202979-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of cyclooctylene bis(piperazinecarboxylates) and analogs as tryptase inhibitors)

RN 202979-16-6 HCAPLUS

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L30 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 1997:797284 HCAPLUS

DN 128:111760

TI Thrombin-like enzyme from Lachesis muta muta venom: isolation and topographical analysis of its active site structure by means of the binding of amidines and guanidines as competitive inhibitors

AU Magalhaes, Arinos; Monteiro, Marcio Ribeiro; Magalhaes, Henrique P. B.; Mares-Guia, Marcos; Rogana, Edyr

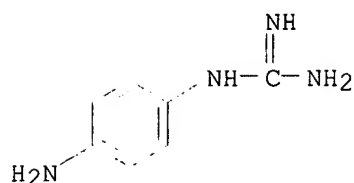
CS Centro de Pesquisa e Desenvolvimento, Fundacao Ezequiel Dias, Belo Horizonte, Brazil

SO Toxicon (1997), 35(10), 1549-1559
 CODEN: TOXIA6; ISSN: 0041-0101

PB Elsevier Science Ltd.

DT Journal

LA English
 CC 4-5 (Toxicology)
 AB Modifications to the purifn. procedure for the title venom were reported. A series of amidine and guanidine derivs. was tested as enzyme inhibitors to gain insight into the mechanism of inhibitor binding and the topog. of the active site.
 ST thrombin enzyme Lachesis venom inhibitor
 IT Enzyme kinetics
 (of inhibition; thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT Venoms
 (snake; thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT Lachesis muta muta
 (thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT Amidines
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT Enzymes, biological studies
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
 (thrombin-like; thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT 113-00-8, Guanidine 113-00-8D, Guanidine, derivs. 143-37-3, Acetamidine 471-29-4, Methylguanidine 618-39-3, Benzamidine 2002-16-6, Phenylguanidine 2339-59-5, 4-Fluorobenzamidine 3459-66-3, 3-Aminobenzamidine 3459-99-2, 3-Nitrobenzamidine 3858-83-1, 4-Aminobenzamidine 5651-14-9, 2-Naphthamidine 14948-83-5, Cyclohexylguanidine 15535-95-2, 4-Carboxybenzamidine 15676-12-7, 4-Carboethoxybenzamidine 18465-11-7, 4-Methylbenzamidine 18465-28-6, 3-Methylbenzamidine 18905-24-3 19563-04-3, 4-Chlorobenzamidine 22265-36-7 22265-37-8, 4-Methoxybenzamidine 25412-75-3, 4-Nitrobenzamidine 69491-64-1, 3-Fluorobenzamidine
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 IT 18905-24-3
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (thrombin-like enzyme from Lachesis muta muta venom isolation and topog. anal. of active site structure by means of binding of amidines and guanidines as competitive inhibitors)
 RN 18905-24-3 HCAPLUS
 CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L30 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 1997:541857 HCAPLUS

DN 127:205895

TI Compositions and methods for treating mast-cell mediated conditions

IN Lum, Robert T.; Gschwend, Heinz W.; Bauer, Barr E.; Kuo, Elaine; Rice, Ken

PA Arris Pharmaceutical Corp., USA

SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 252,099.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-335

ICS A61K031-27; C07C271-06; C07C237-20

NCL 514467000

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5656660	A	19970812	US 1995-455286	19950531 <--
PRAI	US 1994-252099		19940601 <--		
OS	MARPAT 127:205895				
AB	<p>Comps. Z-(X1)n1-X2-X3-X4-(X5)n5-Y-(X'5)n'5-X'4-X'3-X'2-(X'1)n'1-Z' [Y = (un)substituted aryl; Z, Z' = aminomethyl- or guanyl-substituted Ph, cyclohexadienyl, cyclohexenyl, or cyclohexyl; X1, X'1, X5, X'5 = (un)substituted methylene; n1, n'1, n5, n'5 = 0 or 1; X2, X'2, X4, X'4 = NHCO, NHCONH, NHCO2, CONH, O2CNH or N-substituted derivs.; X3, X'3 = (un)substituted cycloalkylene, cycloheteroalkylene, alkylene] were prepd. for the treatment of mast cell mediated inflammatory conditions, such as conjunctivitis, asthma and allergic rhinitis. The comps. for treating mast cell mediated inflammatory conditions include oral, inhalant and topical preps. as well as devices comprising such preps. Thus, bis(p-xylylenediammoniumglycine)-1,4-benzenedimethanol dicarbamate bistrifluoroacetate was prepd. and assayed in vitro for inhibition of tryptase (Ki = 0.56 nM).</p>				
ST	amino acid compd prepn inhibitor tryptase; mast cell tryptase inhibitor prepn				
IT	Nose				
	(allergic rhinitis; comps. and methods for treating mast-cell mediated conditions)				
IT	Anti-inflammatory agents				
	Antiasthmatics				
	Mast cell				
	(comps. and methods for treating mast-cell mediated conditions)				
IT	174958-67-9P	174958-68-0P	174958-69-1P	174958-70-4P	174958-72-6P
	174958-73-7P	174958-74-8P	174958-75-9P	174958-76-0P	174958-77-1P
	174958-79-3P	174958-80-6P	174958-81-7P	174958-82-8P	174958-84-0P
	174958-85-1P	174958-86-2P	174958-87-3P	174958-88-4P	174958-89-5P
	174958-90-8P	174958-91-9P	174958-92-0P	174958-93-1P	174958-94-2P
	174958-95-3P	174958-96-4P	174958-97-5P	174958-98-6P	174958-99-7P
	174959-01-4P	174959-02-5P	174959-03-6P	174959-04-7P	174959-05-8P
	174959-08-1P	174959-10-5P	174959-11-6P	174959-13-8P	174959-14-9P
	174959-15-0P	174959-16-1P	174959-17-2P	174959-18-3P	174959-19-4P

174959-20-7P 174959-21-8P 174959-22-9P 174959-23-0P 174959-24-1P
 174959-25-2P 174959-26-3P 174959-27-4P 174959-28-5P 174959-29-6P
 174959-30-9P 174959-31-0P 174959-32-1P 174959-33-2P 174959-35-4P
 174959-40-1P 174959-41-2P 174959-42-3P 174959-44-5P 174959-45-6P
 174959-46-7P 174959-47-8P 174959-48-9P 175133-76-3P 175133-77-4P
 194659-42-2P 194659-44-4P 194659-45-5P 194659-46-6P 194659-47-7P
 194659-48-8P 194659-49-9P 194659-50-2P 194659-51-3P 194659-52-4P
 194659-53-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(compns. and methods for treating mast-cell mediated conditions)

IT 97501-93-4, Tryptase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(compns. and methods for treating mast-cell mediated conditions)

IT 56-12-2, 4-Aminobutyric acid, reactions 56-40-6, Glycine, reactions
 56-41-7, Alanine, reactions 56-91-7, 4-(Aminomethyl)benzoic acid
 63-91-2, L-Phenylalanine, reactions 100-20-9, 1,4-Benzenedicarbonyl
 dichloride 100-21-0, 1,4-Benzenedicarboxylic acid, reactions 105-10-2
 105-53-3, Diethyl malonate 106-65-0 107-15-3, 1,2-Ethanediamine,
 reactions 107-95-9, .beta.-Alanine 108-30-5, Succinic anhydride,
 reactions 109-76-2, 1,3-Propanediamine 109-90-0, Ethyl isocyanate
 110-60-1, 1,4-Butanediamine 147-85-3, Proline, reactions 338-69-2,
 D-Alanine 420-04-2, Cyanamide 539-48-0, p-Xylylenediamine 589-29-7,
 1,4-Benzenedimethanol 616-34-2, Glycine methyl ester 1013-88-3,
 Benzophenone imine 1119-40-0 1119-48-8 1138-80-3 1197-18-8
 1477-55-0, m-Xylylenediamine 1490-25-1, 3-Carbomethoxypropionyl chloride
 1501-26-4, Methyl glutaryl chloride 4403-71-8, 4-Aminobenzylamine
 5473-12-1, Sarcosine methyl ester 13093-02-2 20580-52-3 37031-29-1
 37517-81-0, Methyl malonyl chloride 174959-86-5 174960-09-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(compns. and methods for treating mast-cell mediated conditions)

IT 5105-78-2P 10362-03-5P 27140-28-9P 27687-14-5P 31417-69-3P
 33233-67-9P 57260-73-8P 68076-36-8P 75178-96-0P 98008-66-3P
 108467-99-8P 108468-00-4P 111623-75-7P 174959-49-0P 174959-50-3P
 174959-51-4P 174959-52-5P 174959-53-6P 174959-54-7P
174959-55-8P 174959-57-0P 174959-58-1P 174959-59-2P
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 174959-81-0P 174959-88-7P 174959-89-8P 174959-90-1P 174959-91-2P
 174959-95-6P 174959-96-7P 174959-97-8P 174959-98-9P 174960-04-4P
 174960-05-5P 174960-06-6P 174960-07-7P 174960-08-8P 194659-54-6P
 194659-55-7P 194659-56-8P 194659-58-0P 194659-59-1P 194659-60-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(compns. and methods for treating mast-cell mediated conditions)

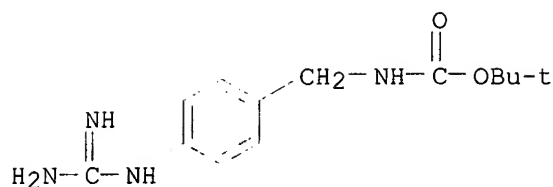
IT **174959-55-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(compns. and methods for treating mast-cell mediated conditions)

RN 174959-55-8 HCAPLUS

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
 1,1-dimethylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

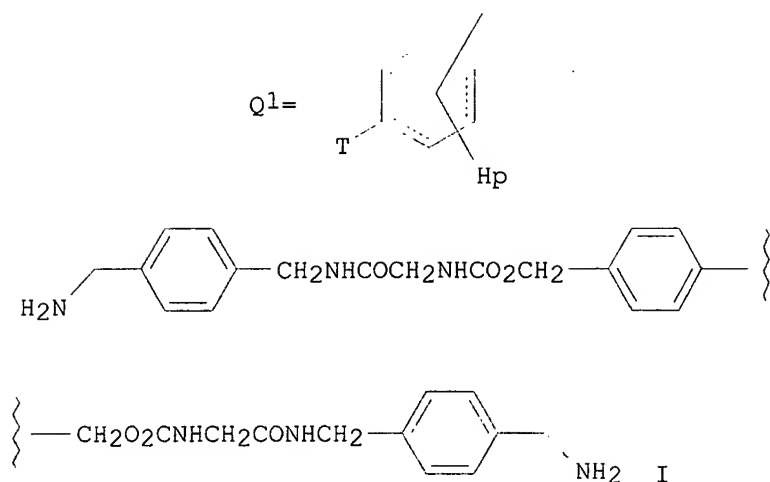
L30 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:202748 HCAPLUS
 DN 124:260612
 TI Preparation of aryl carbamates, -ureas, -guanidines, and related compounds
 for treating mast-cell mediated conditions.
 IN Lum, Robert T.; Gschwend, Heinz W.; Bauer, Barr E.; Kuo, Elaine; Rice, Ken
 PA Arris Pharmaceutical Corp., USA
 SO PCT Int. Appl., 97 pp.
 CODEN: PIXXD2

DT Patent
 LA English

IC ICM C07C279-18
 ICS C07C271-22; C07D207-16; C07C237-34; C07C233-51; C07C275-24;
 A61K031-165; A61K031-16; A61K031-27; A61K031-155; A61K031-17
 CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 1, 34

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9532945	A1	19951207	WO 1995-US6926	19950531 <--
W:			AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT	
RW:			KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG	
AU 9527644	A1	19951221	AU 1995-27644	19950531 <--
EP 763016	A1	19970319	EP 1995-922924	19950531 <--
EP 763016	B1	20000126		
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE	
JP 10501238	T2	19980203	JP 1995-501189	19950531 <--
PRAI US 1994-252099		19940601 <--		
WO 1995-US6926		19950531 <--		
OS MARPAT 124:260612				
GI				



AB Z(X1)mX2X3X4(X5)nY(X15)oX14X13X12(X11)pZ1 [Y = (substituted) aryl; Z, Z1 = Q1; T = CH₂NH₂, NHC(:NH)NH₂; X1, X11, X5, X15 = (substituted) methylene; X2, X12, X4, X14 = NRCO, NRCONR1, NRCO₂, CONR, O₂CNR; R, R1 = H, (substituted) alkyl, aryl, aralkyl; X3, X13 = (substituted) cycloalkylene, cycloheteroalkylene, alkylene; m, n, o, p = 0, 1; q = 4-10], were prepd. Thus, title compd. (I), prepd. by soln. phase couplings, inhibited tryptase from HMC-1 cells with K_i = 0.56 nM.

ST aryl carbamate urea guanidine prepn antiasthmatic; tryptase inhibitor aryl carbamate urea guanidine; allergy inhibitor aryl carbamate urea guanidine; mast cell mediated condition treatment

IT Allergy inhibitors

(prepn. of aryl carbamates, -ureas, -guanidines, and related compds. for treating mast-cell mediated conditions)

IT Bronchodilators

(antiasthmatics, prepn. of aryl carbamates, -ureas, -guanidines, and related compds. for treating mast-cell mediated conditions)

IT 97501-93-4, Tryptase

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(inhibitors; prepn. of aryl carbamates, -ureas, -guanidines, and related compds. for treating mast-cell mediated conditions)

IT	174958-68-0P	174958-69-1P	174958-70-4P	174958-71-5P	174958-72-6P
	174958-73-7P	174958-74-8P	174958-75-9P	174958-76-0P	174958-77-1P
	174958-78-2P	174958-79-3P	174958-80-6P	174958-81-7P	174958-82-8P
	174958-83-9P	174958-84-0P	174958-85-1P	174958-86-2P	174958-87-3P
	174958-88-4P	174958-89-5P	174958-90-8P	174958-91-9P	174958-92-0P
	174958-93-1P	174958-94-2P	174958-95-3P	174958-96-4P	174958-97-5P
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	174959-03-6P	174959-04-7P	174959-05-8P	174959-06-9P	174959-07-0P
	174959-08-1P	174959-09-2P	174959-10-5P	174959-11-6P	174959-12-7P
	174959-13-8P	174959-14-9P	174959-15-0P	174959-16-1P	174959-17-2P
	174959-18-3P	174959-19-4P	174959-20-7P	174959-21-8P	174959-22-9P
	174959-23-0P	174959-24-1P	174959-25-2P	174959-26-3P	174959-27-4P
	174959-28-5P	174959-29-6P	174959-30-9P	174959-32-1P	174959-33-2P
	174959-34-3P	174959-35-4P	174959-36-5P	174959-38-7P	174959-40-1P
	174959-41-2P	174959-42-3P	174959-43-4P	174959-44-5P	174959-45-6P
	174959-46-7P	174959-47-8P	174959-48-9P	175133-76-3P	175133-77-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aryl carbamates, -ureas, -guanidines, and related compds. for treating mast-cell mediated conditions)

IT 56-12-2, 4-Aminobutyric acid, reactions 56-40-6, Glycine, reactions

56-41-7, L-Alanine, reactions 56-91-7, 4-Aminomethylbenzoic acid
 63-91-2, L-Phenylalanine, reactions 75-44-5, Carbonic dichloride
 100-21-0, 1,4-Benzenedicarboxylic acid, reactions 105-53-3, Diethyl
 malonate 106-65-0 107-15-3, 1,2-Ethanediamine, reactions 107-95-9,
 .beta.-Alanine 108-30-5, reactions 109-76-2, 1,3-Diaminopropane
 110-60-1, 1,4-Butanediamine 147-85-3, Proline, reactions 338-69-2,
 D-Alanine 420-04-2, Cyanamide 539-48-0, 1,4-Benzenedimethanamine
 589-29-7, 1,4-Benzenedimethanol 616-34-2, Glycine methyl ester
 1013-88-3, Benzophenone imine 1119-40-0, Dimethyl glutarate 1138-80-3
 1197-18-8, trans-4-Aminomethylcyclohexanecarboxylic acid 1477-55-0,
 m-Xylylenediamine 1490-25-1, 3-Carbomethoxypropionyl chloride
 1501-26-4 2549-93-1, 1,4-Cyclohexanedimethanamine 2579-20-6,
 1,3-Cyclohexanebismethylamine 2949-22-6, Ethyl isocyanatoacetate
 4403-71-8, 4-Aminobenzylamine 5473-12-1, Sarcosine methyl ester
 20580-52-3 37031-29-1 37517-81-0, Methyl malonyl chloride 98008-66-3
 174960-09-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of aryl carbamates, -ureas, -guanidines, and related compds.
 for treating mast-cell mediated conditions)

IT 5105-78-2P 10362-03-5P 27140-28-9P 27687-14-5P 31417-69-3P
 33233-67-9P 57260-73-8P 68076-36-8P 75178-96-0P 94838-55-8P
 108467-99-8P 108468-00-4P 174958-67-9P 174959-49-0P 174959-50-3P
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174959-55-8P 174959-57-0P 174959-58-1P 174959-59-2P
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 174959-70-7P 174959-71-8P 174959-72-9P 174959-73-0P 174959-74-1P
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 174960-02-2P 174960-03-3P 174960-04-4P 174960-05-5P 174960-06-6P
 174960-07-7P 174960-08-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of aryl carbamates, -ureas, -guanidines, and related compds.
 for treating mast-cell mediated conditions)

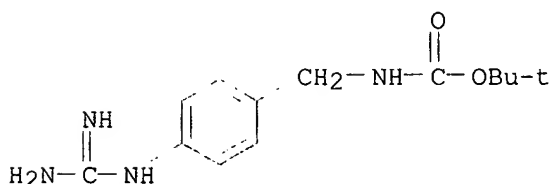
IT **174959-55-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of aryl carbamates, -ureas, -guanidines, and related compds.
 for treating mast-cell mediated conditions)

RN 174959-55-8 HCAPLUS

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-,
 1,1-dimethylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



HCl

AN 1985:181546 HCAPLUS
 DN 102:181546
 TI Separation of low-molecular-weight and high-molecular-weight urokinases
 PA Wakamoto Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C12N009-72
 CC 7-2 (Enzymes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 60006191	A2	19850112	JP 1983-96970	19830602 <--
	JP 62030755	B4	19870703		
PRAI	JP 1983-96970		19830602	<--	

AB High-mol.-wt. urokinase is sepd. from low-mol.-wt. urokinase by adsorption chromatog. with adsorbent gels contg. -NH(CH₂)₅COOH and -NH(CH₂)₅CONHC₆H₄R (R = amidino or guanidino) groups. Thus, CNBr-activated Sepharose CL-6B was reacted with 6-aminocaproic acid and then reacted with CMC and p-aminobenzamidine to obtain a gel prepn. contg. 6-aminocaproic acid 61.7 and p-aminobenzamidine 22.5 .mu.mol/mL gel. When a crude urokinase prepn. (specific activity 7200 IU/mg protein) was chromatographed on this gel and eluted with a 0.1M phosphate buffer (pH 7.0) contg. 1M NaCl, low-mol.-wt. urokinase with a specific activity of 142,000 IU/mg protein was recovered. Further elution with a 0.2-0.55M NaCl-contg. buffer at pH 4.0 recovered pyrogen-free high-mol.-wt. urokinase with a specific activity of 127,000 IU/mg protein at 85% yield.

ST urokinase multiple form sepn affinity chromatog

IT 9039-53-6

RL: BIOL (Biological study)

(multiple forms of, affinity chromatog. sepn. of)

IT 60-32-2D, Sepharose complexes 3858-83-1D, aminocaproate-Sepharose complexes 18905-24-3D, aminocaproate-Sepharose complexes

RL: BIOL (Biological study)

(urokinase multiple forms sepn. on)

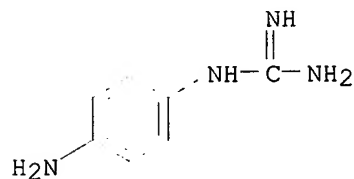
IT 18905-24-3D, aminocaproate-Sepharose complexes

RL: BIOL (Biological study)

(urokinase multiple forms sepn. on)

RN 18905-24-3 HCAPLUS

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L30 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2003 ACS

AN 1985:108930 HCAPLUS

DN 102:108930

TI Adsorbents for purification of enzymes

PA Wakamoto Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

IC C12N009-00; C12N009-72

CC 7-2 (Enzymes)

Section cross-reference(s): 9

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59187779	A2	19841024	JP 1983-61028	19830408 <--
	JP 61048918	B4	19861027		
PRAI	JP 1983-61028		19830408	<--	

AB A new type of adsorbent for affinity chromatog. of enzymes, esp. urokinase, is prepd. by modification of conventional H₂O-insol. carriers with the spacer 6-aminocaproic acid; 25-65% of the carboxyl moieties of the carrier-bound spacer are further modified with p-aminobenzamidine or p-aminophenylguanidine. Thus, 20 mL CNBr-activated Sepharose CL-6B was reacted with 2 g 6-aminocaproic acid at 20.degree. for 10 h and the product was further reacted with p-aminobenzamidine in the presence of a condensation agent at pH 4.2-4.6 for 12 h to obtain a modified carrier in which the ratio of bound spacer (6-aminocaproic acid) to aminobenzamidine-modified spacer was 70:30. When a crude urokinase prepn. (specific activity 3500 IU/mg protein) was applied to a column packed with the modified Sepharose and eluted with a 0.1M phosphate buffer contg. 0.4M NaCl, purified urokinase with specific activity of 115,000 IU/mg protein was obtained at 35% yield; the purified urokinase thus obtained showed a neg. pyrogen test.

ST urokinase purifn Sepharose affinity chromatog; affinity chromatog
Sepharose enzyme

IT Enzymes

RL: PROC (Process)

(affinity chromatog. of, on aminobenzamidine- and aminophenylguanidine-contg. Sepharose derivs.)

IT Chromatography, column and liquid

(affinity, of urokinase and other enzymes, on aminobenzamidine- and aminophenylguanidine-contg. Sepharose derivs.)

IT 9039-53-6

RL: PROC (Process)

(affinity chromatog. of, on aminobenzamidine-modified Sepharose)

IT 55128-01-3DP, benzamidine derivs.

RL: PREP (Preparation)

(prepn. of and urokinase and other enzymes affinity chromatog. on)

IT 55128-01-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminobenzamidine and aminophenylguanidine)

IT 62610-50-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminocaproate)

IT 3858-83-1 18905-24-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminocaproic acid-Sepharose)

IT 60-32-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with cyanogen-bromide-activated Sepharose CL-6B)

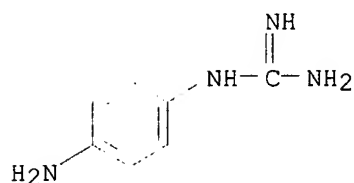
IT 18905-24-3

RL: RCT (Reactant); RACT (Reactant or reagent)

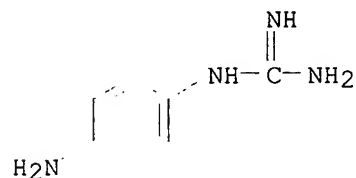
(reaction of, with aminocaproic acid-Sepharose)

RN 18905-24-3 HCAPLUS

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)

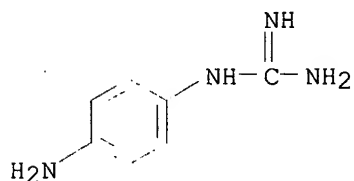


L30 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2003 ACS
 AN 1973:94208 HCAPLUS
 DN 78:94208
 TI Affinity chromatography. Purification of bovine trypsin and thrombin
 AU Hixson, H. F., Jr.; Nishikawa, A. H.
 CS Rochester Res. Cent., Xerox Corp., Webster, NY, USA
 SO Archives of Biochemistry and Biophysics (1973), 154(2), 501-9
 CODEN: ABBIA4; ISSN: 0003-9861
 DT Journal
 LA English
 CC 7-2 (Enzymes)
 AB Bovine trypsin was purified by affinity chromatog. on agarose beads contg. covalently bound p-aminophenylguanidine, p-aminobenzamidine, or m-aminobenzamidine. Bovine thrombin was purified on a m-aminobenzamidine-agarose column contg. a high concn. of the inhibitor. The values of the inhibition const., K_i , for these inhibitors were detd. for both enzymes, and inhibition was 5-10 times poorer for thrombin than for trypsin. Only those benzamidines with low K_i values and coupled in high concn. to the agarose matrix were satisfactory for thrombin purifn. Affinity-purified trypsin and thrombin were both >90% active as measured by active site titrn.
 ST affinity chromatog trypsin thrombin; benzamidine affinity chromatog trypsin
 IT 9002-04-4 9002-07-7
 RL: PROC (Process)
 (affinity chromatog. of)
 IT 618-39-3 3459-66-3 3858-83-1 18905-24-3 40642-34-0
 RL: BIOL (Biological study)
 (as enzyme affinity chromatog. ligand)
 IT 2002-16-6
 RL: BIOL (Biological study)
 (as enzyme affinity chromatog. ligand)
 IT 18905-24-3
 RL: BIOL (Biological study)
 (as enzyme affinity chromatog. ligand)
 RN 18905-24-3 HCAPLUS
 CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L30 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2003 ACS
 AN 1968:503313 HCAPLUS
 DN 69:103313

TI 4-Guanidinobenzoic acid benzyl ester and 4-guanidinobenzoic acid
4'-nitrobenzyl ester: two new potent inhibitors of trypsin
AU Mix, Hermann; Trettin, Hans Joachim; Guelzow, Martin
CS Deut. Akad. Wiss. Berlin, Rostock, Ger. Dem. Rep.
SO Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1968),
349(9), 1237-8
CODEN: HSZPAZ; ISSN: 0018-4888
DT Journal
LA German
CC 3 (Enzymes)
AB 4-Guanidinobenzoic acid benzyl ester and 4-guanidinobenzoic acid
4'-nitrobenzyl ester inhibited the tryptic cleavage of
N.alpha.-benzoylarginine p-nitroanilide with resp. inhibitor consts. of
8.7 and 3.25 .times. 10⁻⁷M. The corresponding consts. for the inhibition
of the autocatalytic activation of trypsinogen were 4.8 and 3.2 .times.
10⁻⁸M, resp. The inhibitor consts. for the inhibition of tryptic cleavage
of N.alpha.-benzoylarginine p-nitroanilide (and autocatalytic activation
of trypsinogen) were detd. for the following compds.: 4-amidinobenzoic
acid benzyl ester 7.05 .times. 10⁻⁶M (5.75 .times. 10⁻⁶M), phenylguanidine
8.75 .times. 10⁻⁵M (2.54 .times. 10⁻⁵M), benzamidine 2.4 .times. 10⁻⁵M
(6.85 .times. 10⁻⁶M), 4-aminobenzamidine 1.05 .times. 10⁻⁵M (3.48 .times.
10⁻⁶M), 4-aminophenylguanidine, 3.12 .times. 10⁻⁴M (6.7 .times. 10⁻⁵M),
4-guanidinobenzoic acid, 1.6 .times. 10⁻⁴M (5.9 .times. 10⁻⁵M), and
4-amidinobenzoic acid, 1.09 .times. 10⁻⁴M (3.1 .times. 10⁻⁵M).
ST guanidinobenzoates trypsin; trypsin guanidinobenzoates; benzoylarginine
trypsin; amidinobenzoates trypsin; phenylguanidine trypsin
IT 9002-07-7, Trypsin, reactions 9002-08-8, Trypsinogen
(inhibition of, by phenylguanidine and benzamidine derivs.)
IT 618-39-3 2002-16-6 3858-83-1 14209-67-7 15535-95-2 16060-65-4
18905-21-0 18905-22-1 **18905-24-3**
RL: BIOL (Biological study)
(trypsin and trypsinogen inhibition by, kinetics of)
IT **18905-24-3**
RL: BIOL (Biological study)
(trypsin and trypsinogen inhibition by, kinetics of)
RN 18905-24-3 HCAPLUS
CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



=> fil uspatall

FILE 'USPATFULL' ENTERED AT 10:55:55 ON 14 FEB 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 10:55:55 ON 14 FEB 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr tot 128

L28 ANSWER 1 OF 5 USPATFULL
AN 2002:251830 USPATFULL
TI Potassium channel blocking agents
IN Jensen, Bo Skaaning, Copenhagen S, DENMARK

Olesen, Soren Peter, Klampenborg, DENMARK
 Teuber, Lene, Vaerloose, DENMARK
 Peters, Dan, Arlov, SWEDEN
 Strobaek, Dorte, Farum, DENMARK
 PA NeuroSearch A/S (non-U.S. corporation)
 PI US 2002137784 A1 20020926
 AI US 2002-84179 A1 20020228 (10)
 RLI Division of Ser. No. US 2000-750345, filed on 29 Dec 2000, GRANTED, Pat.
 No. US 6380180
 PRAI DK 1998-865 19980702
 DT Utility
 FS APPLICATION
 LREP BIRCH STEWART KOLASCH & BIRCH, PO BOX 747, FALLS CHURCH, VA, 22040-0747
 CLMN Number of Claims: 34
 ECL Exemplary Claim: 1
 DRWN No Drawings
 LN.CNT 1761

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to novel potassium channel blocking agents, and their use in the preparation of pharmaceutical compositions.

Moreover the invention is directed to pharmaceutical compositions useful for the treatment or alleviation of diseases or disorders associated with the activity of potassium channels, in particular asthma, cystic fibrosis, chronic obstructive pulmonary disease and rhinorrhea, convulsions, vascular spasms, coronary artery spasms, renal disorders, polycystic kidney disease, bladder spasms, urinary incontinence, bladder outflow obstruction, irritable bowel syndrome, gastrointestinal dysfunction, secretory diarrhoea, ischaemia, cerebral ischaemia, ischaemic hearth disease, angina pectoris, coronary hearth disease, traumatic brain injury, psychosis, anxiety, depression, dementia, memory and attention deficits, Alzheimer's disease, dysmenorrhea, narcolepsy, Reynaud's disease, intermittent claudication, Sjorgren's syndrome, migraine, arrhythmia, hypertension, absence seizures, myotonic muscle dystrophias, xerostomia, diabetes type II, hyperinsulinemia, premature labor, baldness, cancer, and immune suppression.

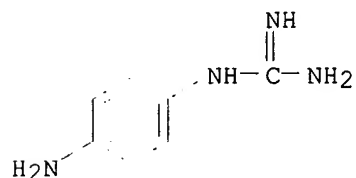
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 18905-24-3P

(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)

RN 18905-24-3 USPATFULL

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 5 USPATFULL

AN 2002:92721 USPATFULL

TI Potassium channel blocking agents

IN Jensen, Bo Skaaning, Copenhagen S, DENMARK

Olesen, Soren Peter, Klampenborg, DENMARK

Teuber, Lene, Vaerloose, DENMARK

Peters, Dan, Arlov, SWEDEN

Strobaek, Dorte, Farum, DENMARK

PA NeuroSearch A/S (non-U.S. corporation)
 PI US 2002049246 A1 20020425
 US 6380180 B2 20020430
 AI US 2000-750345 A1 20001229 (9)
 RLI Division of Ser. No. US 1999-347514, filed on 2 Jul 1999, GRANTED, Pat.
 No. US 6194447
 PRAI DK 1998-865 19980702
 US 1998-92218P 19980708 (60)
 DT Utility
 FS APPLICATION
 LREP BIRCH STEWART KOLASCH & BIRCH, PO BOX 747, FALLS CHURCH, VA, 22040-0747
 CLMN Number of Claims: 34
 ECL Exemplary Claim: 1
 DRWN No Drawings
 LN.CNT 1769

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to novel potassium channel blocking agents, and their use in the preparation of pharmaceutical compositions.

Moreover the invention is directed to pharmaceutical compositions useful for the treatment or alleviation of diseases or disorders associated with the activity of potassium channels, in particular asthma, cystic fibrosis, chronic obstructive pulmonary disease and rhinorrhea, convulsions, vascular spasms, coronary artery spasms, renal disorders, polycystic kidney disease, bladder spasms, urinary incontinence, bladder outflow obstruction, irritable bowel syndrome, gastrointestinal dysfunction, secretory diarrhoea, ischaemia, cerebral ischaemia, ischaemic heart disease, angina pectoris, coronary heart disease, traumatic brain injury, psychosis, anxiety, depression, dementia, memory and attention deficits, Alzheimer's disease, dysmenorrhea, narcolepsy, Reynaud's disease, intermittent claudication, Sjorgren's syndrome, migraine, arrhythmia, hypertension, absence seizures, myotonic muscle dystrophy, xerostomi, diabetes type II, hyperinsulinemia, premature labor, baldness, cancer, and immune suppression.

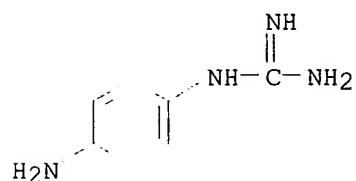
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 18905-24-3P

(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)

RN 18905-24-3 USPATFULL

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 3 OF 5 USPATFULL

AN 2001:29599 USPATFULL

TI Bis (benzimidazole) derivatives serving as potassium blocking agents

IN Jensen, Bo Skaaning, Copenhagen S, Denmark

Olesen, S.o slashed.ren Peter, Klampenborg, Denmark

Teuber, Lene, V.ae buttet.rl.o slashed.se, Denmark

Peters, Dan, Arlov, Denmark

Str.o slashed.b.ae buttet.k, Dorte, Farum, Denmark

PA Neurosearch A/S, Ballerup, Denmark (non-U.S. corporation)

PI US 6194447 B1 20010227

AI US 1999-347514 19990702 (9)
 PRAI DK 1998-865 19980702
 US 1998-92218P 19980708 (60)
 DT Utility
 FS Granted
 EXNAM Primary Examiner: Stockton, Laura L.
 LREP Birch, Stewart, Kolasch & Birch, LLP
 CLMN Number of Claims: 5
 ECL Exemplary Claim: 1
 DRWN No Drawings
 LN.CNT 1529

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to novel potassium channel blocking agents, and their use in the preparation of pharmaceutical compositions.

Moreover the invention is directed to pharmaceutical compositions useful for the treatment or alleviation of diseases or disorders associated with the activity of potassium channels, in particular asthma, cystic fibrosis, chronic obstructive pulmonary disease and rhinorrhea, convulsions, vascular spasms, coronary artery spasms, renal disorders, polycystic kidney disease, bladder spasms, urinary incontinence, bladder outflow obstruction, irritable bowel syndrome, gastrointestinal dysfunction, secretory diarrhoea, ischaemia, cerebral ischaemia, ischaemic heart disease, angina pectoris, coronary heart disease, traumatic brain injury, psychosis, anxiety, depression, dementia, memory and attention deficits, Alzheimer's disease, dysmenorrhea, narcolepsy, Reynaud's disease, intermittent claudication, Sjorgren's syndrome, migraine, arrhythmia, hypertension, absence seizures, myotonic muscle dystrophia, xerostomi, diabetes type II, hyperinsulinemia, premature labor, baldness, cancer, and immune suppression.

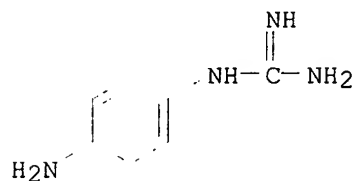
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 18905-24-3P

(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)

RN 18905-24-3 USPATFULL

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 5 USPATFULL

AN 97:71094 USPATFULL

TI Compositions and methods for treating mast-cell mediated conditions

IN Lum, Robert T., Palo Alto, CA, United States
 Gschwend, Heinz W., Belmont, CA, United States
 Bauer, Barr E., Foster City, CA, United States
 Kuo, Elaine, San Francisco, CA, United States
 Rice, Ken, Redwood City, CA, United States

PA Arris Pharmaceutical Corporation, South San Francisco, CA, United States
 (U.S. corporation)

PI US 5656660 19970812

AI US 1995-455286 19950531 (8)

RLI Continuation-in-part of Ser. No. US 1994-252099, filed on 1 Jun 1994

DT Utility

FS Granted
 EXNAM Primary Examiner: Conrad, Joseph
 LREP Townsend and Townsend and Crew LLP
 CLMN Number of Claims: 42
 ECL Exemplary Claim: 1
 DRWN 5 Drawing Figure(s); 3 Drawing Page(s)
 LN.CNT 2676

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention describes compounds, methods and compositions effective to treat mast cell mediated inflammatory conditions, such as conjunctivitis, asthma and allergic rhinitis. The compounds of the invention comprise novel mono- and di-aminomethylbenzyl, aminobenzyl, guanidylbenzyl and benzyl tryptase inhibitors. The compositions for treating mast cell mediated inflammatory conditions include oral, inhalant and topical preparations as well as devices comprising such preparations.

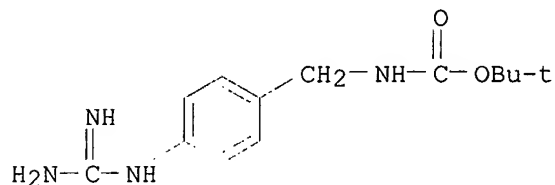
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 174959-55-8P

(compns. and methods for treating mast-cell mediated conditions)

RN 174959-55-8 USPATFULL

CN Carbamic acid, [[4-[(aminoiminomethyl)amino]phenyl]methyl]-, 1,1-dimethylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L28 ANSWER 5 OF 5 USPAT2
 AN 2002:92721 USPAT2
 TI Potassium channel blocking agents
 IN Jensen, Bo Skaaning, Copenhagen S, DENMARK
 Olesen, S.o slashed.ren Peter, Klampenborg, DENMARK
 Teuber, Lene, Vaerl.o slashed.se, DENMARK
 Peters, Dan, Arlov, SWEDEN
 Str.o slashed.baek, Dorte, Farum, DENMARK
 PA NeuroSearch A/S, Ballerup, DENMARK (non-U.S. corporation)
 PI US 6380180 B2 20020430
 AI US 2000-750345 20001229 (9)
 RLI Division of Ser. No. US 1999-347514, filed on 2 Jul 1999, now patented,
 Pat. No. US 6194447
 PRAI DK 1998-865 19980702
 US 1998-92218P 19980708 (60)
 DT Utility
 FS GRANTED
 EXNAM Primary Examiner: Stockton, Laura L.
 LREP Birch, Stewart, Kolasch & Birch, LLP
 CLMN Number of Claims: 9
 ECL Exemplary Claim: 1
 DRWN 0 Drawing Figure(s); 0 Drawing Page(s)
 LN.CNT 1535
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to novel potassium channel blocking agents, and their use in the preparation of pharmaceutical compositions.

Moreover the invention is directed to pharmaceutical compositions useful for the treatment or alleviation of diseases or disorders associated with the activity of potassium channels, in particular asthma, cystic fibrosis, chronic obstructive pulmonary disease and rhinorrhea, convulsions, vascular spasms, coronary artery spasms, renal disorders, polycystic kidney disease, bladder spasms, urinary incontinence, bladder outflow obstruction, irritable bowel syndrome, gastrointestinal dysfunction, secretory diarrhoea, ischaemia, cerebral ischaemia, ischaemic heart disease, angina pectoris, coronary heart disease, traumatic brain injury, psychosis, anxiety, depression, dementia, memory and attention deficits, Alzheimer's disease, dysmenorrhea, narcolepsy, Reynaud's disease, intermittent claudication, Sjorgren's syndrome, migraine, arrhythmia, hypertension, absence seizures, myotonic muscle dystrophia, xerostomi, diabetes type II, hyperinsulinemia, premature labor, baldness, cancer, and immune suppression.

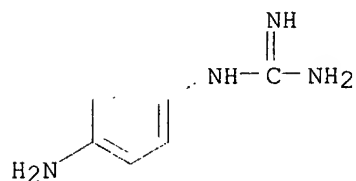
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 18905-24-3P

(prepn. of aminobenzimidazoles and guanidines as potassium channel blocking agents)

RN 18905-24-3 USPAT2

CN Guanidine, (4-aminophenyl)- (9CI) (CA INDEX NAME)



=> fil reg

FILE 'REGISTRY' ENTERED AT 11:45:19 ON 14 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

DICTIONARY FILE UPDATES: 12 FEB 2003 HIGHEST RN 489395-53-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

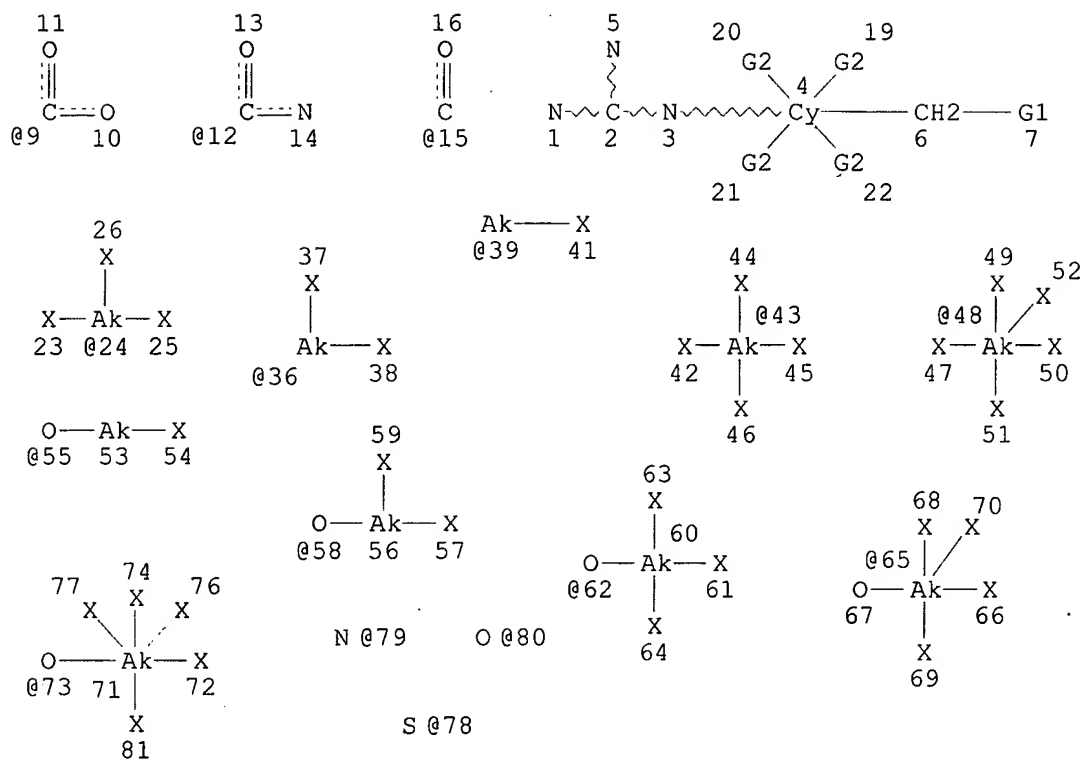
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 144

L38

STR



VAR G1=79/80/78/9/12/15
 VAR G2=H/AK/39/36/24/43/48/55/58/62/65/73

NODE ATTRIBUTES:

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 CONNECT IS M1 RC AT 14
 CONNECT IS M1 RC AT 15
 CONNECT IS M1 RC AT 78
 CONNECT IS M1 RC AT 79
 CONNECT IS M1 RC AT 80

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY AT 4

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 67

STEREO ATTRIBUTES: NONE

L40 SCR 1433

L42 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 O
 R 2043 OR 2054

L44 1495 SEA FILE=REGISTRY CSS FUL L38 AND L40 NOT L42

100.0% PROCESSED 380947 ITERATIONS

1495 ANSWERS

SEARCH TIME: 00.00.48

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L44 1495 S L38 AND L40 NOT L42 CSS FUL

SAV L9 KUMAR049/A

SAV L44 KUMAR049A/A
L45 1475 S L44 NOT L9
L46 1 S L9 NOT L44
SAV L45 KUMAR049B/A

FILE 'REGISTRY' ENTERED AT 11:45:19 ON 14 FEB 2003

=> fil reg

FILE 'REGISTRY' ENTERED AT 15:12:59 ON 14 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2003 HIGHEST RN 490012-70-9

DICTIONARY FILE UPDATES: 13 FEB 2003 HIGHEST RN 490012-70-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

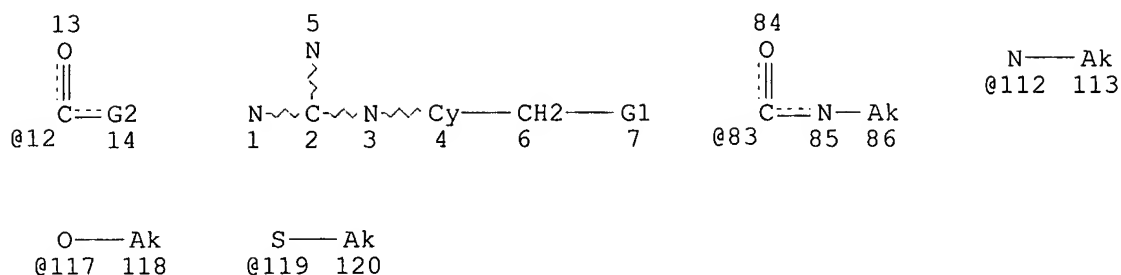
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STN Note 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 127

L1 (33)SEA FILE=REGISTRY ABB=ON PLU=ON (139639-24-0/BI OR 152120-54-
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327973-70-6/BI OR 327973-71-7/BI OR 327973-72-8/BI OR 327973-73
-9/BI OR 327973-74-0/BI OR 327973-75-1/BI OR 327973-76-2/BI OR
327973-77-3/BI OR 327973-78-4/BI OR 327973-79-5/BI OR 4403-71-8
/BI OR 4411-25-0/BI OR 4457-32-3/BI OR 94838-55-8/BI)
L2 (27)SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND N>=3
L3 (6)SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND (C24H24N4O4 OR
C29H32N4O6 OR C18H16F3N3O6S OR C14H22N4O4 OR C26H34N4O6 OR
C18H28N4O4)
L4 (21)SEA FILE=REGISTRY ABB=ON PLU=ON L2 NOT L3
L5 (18)SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND 1/NC
L6 (15)SEA FILE=REGISTRY ABB=ON PLU=ON L1 NOT L5
L7 (3)SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (C19H27N5O OR
C13H20N4O2 OR C16H17N5O4)
L8 (21)SEA FILE=REGISTRY ABB=ON PLU=ON (L5 OR L7)
L9 STR



VAR G1=OH/NH2/112/SH/117/119/83/12

VAR G2=OH/NH2

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 4

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY AT 4

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L27 32 SEA FILE=REGISTRY SUB=L13 CSS FUL L26

100.0% PROCESSED 1475 ITERATIONS

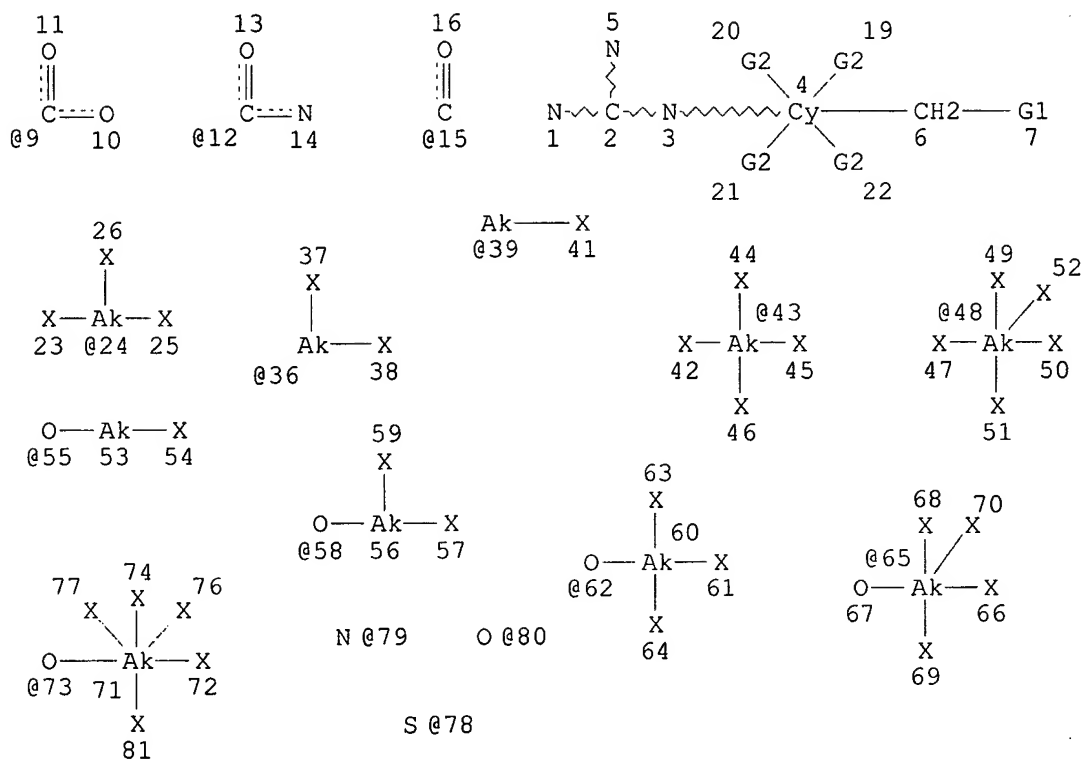
32 ANSWERS

SEARCH TIME: 00.00.01

=> d sta que 130

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L1 ( 33)SEA FILE=REGISTRY ABB=ON PLU=ON (139639-24-0/BI OR 152120-54-
    2/BI OR 168050-39-3/BI OR 172348-93-5/BI OR 172348-94-6/BI OR
    174959-55-8/BI OR 174959-56-9/BI OR 18905-24-3/BI OR 202979-16-
    6/BI OR 207857-19-0/BI OR 282718-33-6/BI OR 282718-34-7/BI OR
    282718-36-9/BI OR 282718-37-0/BI OR 282718-40-5/BI OR 282718-42-
    7/BI OR 282718-45-0/BI OR 327971-04-0/BI OR 327973-69-3/BI OR
    327973-70-6/BI OR 327973-71-7/BI OR 327973-72-8/BI OR 327973-73-
    9/BI OR 327973-74-0/BI OR 327973-75-1/BI OR 327973-76-2/BI OR
    327973-77-3/BI OR 327973-78-4/BI OR 327973-79-5/BI OR 4403-71-8
    /BI OR 4411-25-0/BI OR 4457-32-3/BI OR 94838-55-8/BI)
L2 ( 27)SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND N>=3
L3 ( 6)SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND (C24H24N4O4 OR
    C29H32N4O6 OR C18H16F3N3O6S OR C14H22N4O4 OR C26H34N4O6 OR
    C18H28N4O4)
L4 ( 21)SEA FILE=REGISTRY ABB=ON PLU=ON L2 NOT L3
L5 ( 18)SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND 1/NC
L6 ( 15)SEA FILE=REGISTRY ABB=ON PLU=ON L1 NOT L5
L7 ( 3)SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (C19H27N5O OR
    C13H20N4O2 OR C16H17N5O4)
L8 ( 21)SEA FILE=REGISTRY ABB=ON PLU=ON (L5 OR L7)
L9 STR
  
```



```
VAR G1=79/80/78/9/12/15
VAR G2=H/AK/39/36/24/43/48/55/58/62/65/73
```

NODE ATTRIBUTES:

CONNECT	IS	M1	RC	AT	10
CONNECT	IS	M1	RC	AT	14
CONNECT	IS	M1	RC	AT	15
CONNECT	IS	M1	RC	AT	78
CONNECT	IS	M1	RC	AT	79
CONNECT	IS	M1	RC	AT	80

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY AT 4

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 67

STEREO ATTRIBUTES: NONE

L10 SCR 1433

L11 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 O

R 2043 OR 2054

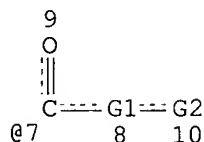
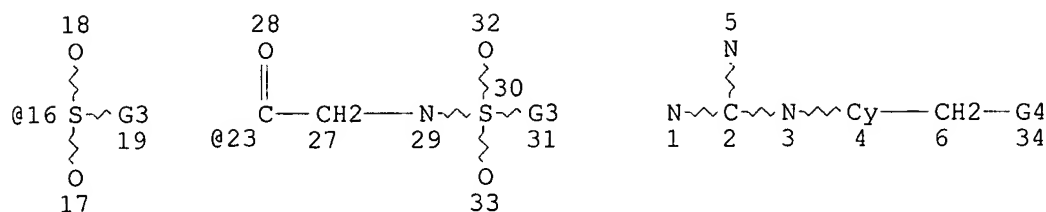
L12 (1495)SEA FILE=REGISTRY CSS FUL L9 AND L10 NOT L11

```

L13      1475 SEA FILE=REGISTRY ABB=ON  PLU=ON  L12 NOT L8

```

L28 STR



VAR G1=O/N
 VAR G2=H/AK/CY/16
 VAR G3=H/AK/CY
 VAR G4=7/23
 NODE ATTRIBUTES:
 CONNECT IS M1 RC AT 4
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY AT 4
 DEFAULT ECLEVEL IS LIMITED

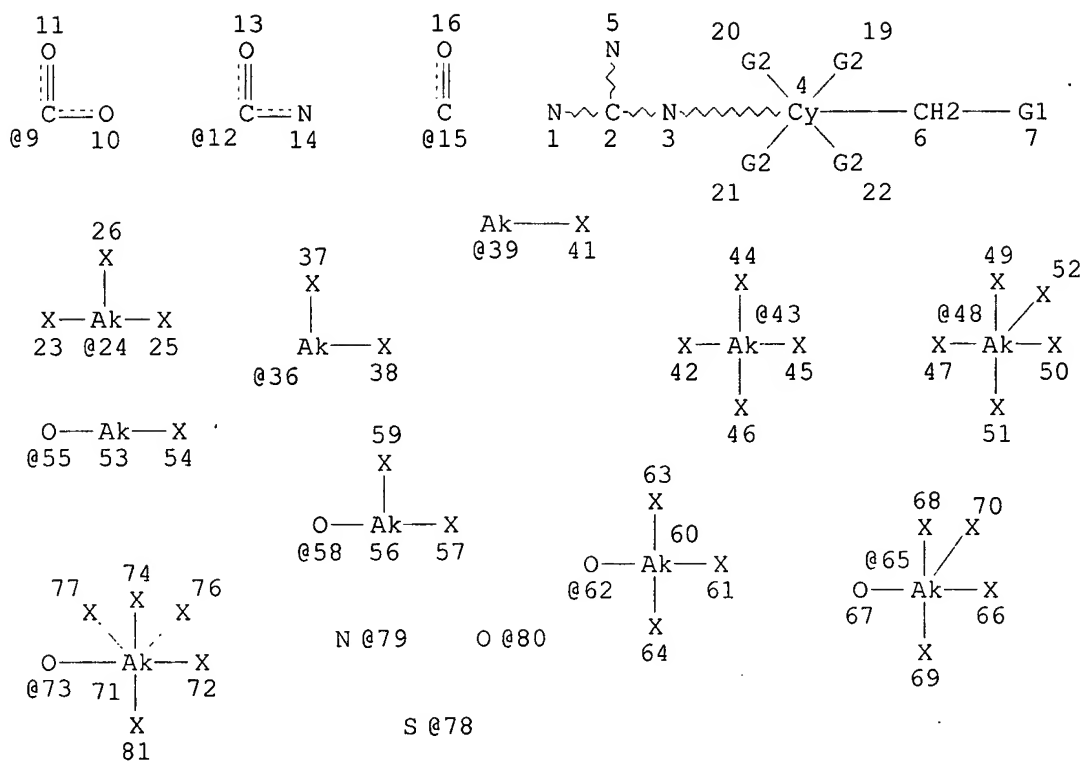
GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
 L30 15 SEA FILE=REGISTRY SUB=L13 CSS FUL L28

100.0% PROCESSED 1033 ITERATIONS 15 ANSWERS
 SEARCH TIME: 00.00.01

=> d sta que 133

L1 (33)SEA FILE=REGISTRY ABB=ON PLU=ON (139639-24-0/BI OR 152120-54-2/BI OR 168050-39-3/BI OR 172348-93-5/BI OR 172348-94-6/BI OR 174959-55-8/BI OR 174959-56-9/BI OR 18905-24-3/BI OR 202979-16-6/BI OR 207857-19-0/BI OR 282718-33-6/BI OR 282718-34-7/BI OR 282718-36-9/BI OR 282718-37-0/BI OR 282718-40-5/BI OR 282718-42-7/BI OR 282718-45-0/BI OR 327971-04-0/BI OR 327973-69-3/BI OR 327973-70-6/BI OR 327973-71-7/BI OR 327973-72-8/BI OR 327973-73-9/BI OR 327973-74-0/BI OR 327973-75-1/BI OR 327973-76-2/BI OR 327973-77-3/BI OR 327973-78-4/BI OR 327973-79-5/BI OR 4403-71-8/BI OR 4411-25-0/BI OR 4457-32-3/BI OR 94838-55-8/BI)
 L2 (27)SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND N>=3
 L3 (6)SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND (C24H24N4O4 OR C29H32N4O6 OR C18H16F3N3O6S OR C14H22N4O4 OR C26H34N4O6 OR C18H28N4O4)
 L4 (21)SEA FILE=REGISTRY ABB=ON PLU=ON L2 NOT L3
 L5 (18)SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND 1/NC
 L6 (15)SEA FILE=REGISTRY ABB=ON PLU=ON L1 NOT L5
 L7 (3)SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (C19H27N5O OR C13H20N4O2 OR C16H17N5O4)
 L8 (21)SEA FILE=REGISTRY ABB=ON PLU=ON (L5 OR L7)
 L9 STR



```
VAR G1=79/80/78/9/12/15
VAR G2=H/AK/39/36/24/43/48/55/58/62/65/73
```

NODE ATTRIBUTES:

CONNECT	IS	M1	RC	AT	10
CONNECT	IS	M1	RC	AT	14
CONNECT	IS	M1	RC	AT	15
CONNECT	IS	M1	RC	AT	78
CONNECT	IS	M1	RC	AT	79
CONNECT	IS	M1	RC	AT	80

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY AT 4

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 67

STEREO ATTRIBUTES: NONE

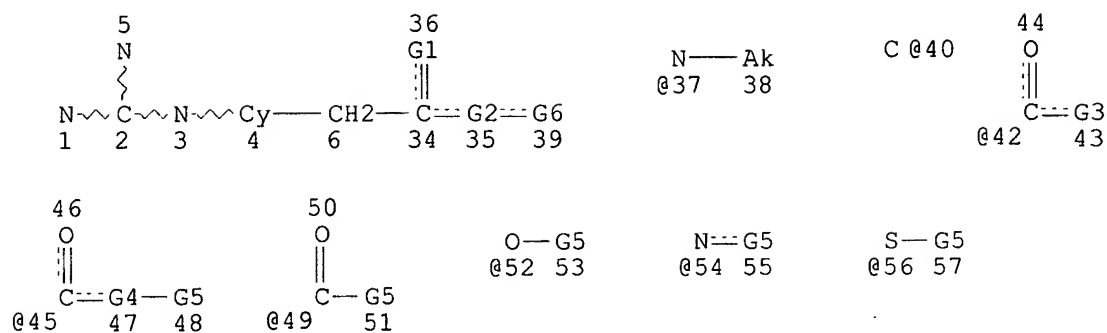
L10 SCR 1433

L11 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 O
R 2043 OR 2054

```
L12 (      1495)SEA FILE=REGISTRY CSS FUL L9 AND L10 NOT L11
```

L13 1475 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT L8

L31 STR



VAR G1=O/S/N/37
 REP G2=(0-2) 40
 VAR G3=OH/NH2
 VAR G4=O/N
 VAR G5=AK/CY
 VAR G6=OH/NH2/SH/CHO/42/45/49/52/54/56

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 4
 CONNECT IS M1 RC AT 40
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY AT 4
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

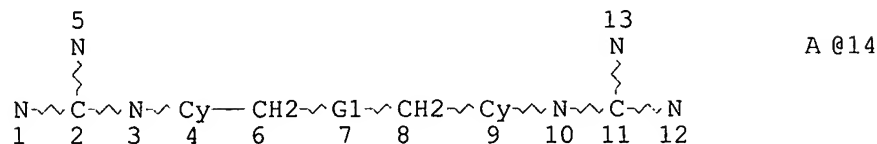
L33 17 SEA FILE=REGISTRY SUB=L13 CSS FUL L31

100.0% PROCESSED 1475 ITERATIONS
 SEARCH TIME: 00.00.01

17 ANSWERS

=> d sta que 155

L50 STR



REP G1=(1-20) 14

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 4
 CONNECT IS M1 RC AT 9
 CONNECT IS M1 RC AT 14
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L53 30 SEA FILE=REGISTRY SSS FUL L50

L54 24 SEA FILE=REGISTRY ABB=ON PLU=ON L53 NOT SQL/FA
 L55 1 SEA FILE=REGISTRY ABB=ON PLU=ON L54 AND C10H14N8S4

=> d his

(FILE 'HOME' ENTERED AT 14:11:36 ON 14 FEB 2003)
 SET COST OFF

FILE 'REGISTRY' ENTERED AT 14:12:02 ON 14 FEB 2003
 ACT KUMAR049B/A

```

L1 ( 33)SEA FILE=REGISTRY ABB=ON PLU=ON (139639-24-0/BI OR 152120-54-
L2 ( 27)SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND N>=3
L3 ( 6)SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND (C24H24N4O4 OR C29H32N
L4 ( 21)SEA FILE=REGISTRY ABB=ON PLU=ON L2 NOT L3
L5 ( 18)SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND 1/NC
L6 ( 15)SEA FILE=REGISTRY ABB=ON PLU=ON L1 NOT L5
L7 ( 3)SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (C19H27N5O OR C13H20N4
L8 ( 21)SEA FILE=REGISTRY ABB=ON PLU=ON (L5 OR L7)
L9 STR
L10 SCR 1433
L11 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 OR 204
L12 ( 1495)SEA FILE=REGISTRY CSS FUL L9 AND L10 NOT L11
L13 1475 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT L8

```

```

L14 STR L9
L15 0 S L14 CSS SAM SUB=L13
L16 1 S L14 SAM SUB=L13
L17 23 S L14 FUL SUB=L13
    SAV L17 KUMAR049C/A
L18 0 S L14 CSS FUL SUB=L17
    SAV L18 KUMAR049D/A
L19 STR L14
L20 STR L19
L21 0 S L20 CSS SAM SUB=L13
L22 0 S L20 CSS FUL SUB=L13
    SAV L22 KUMAR049E/A
    DEL KUMAR049E/A
L23 STR L20
L24 0 S L23 CSS SAM SUB=L13
L25 0 S L23 CSS FUL SUB=L13
    SAV L25 KUMAR049E/A
L26 STR L23
L27 32 S L26 CSS FUL SUB=L13
    DEL KUMAR049E/A
L28 STR L26
L29 2 S L28 CSS SAM SUB=L13
L30 15 S L28 CSS FUL SUB=L13
    SAV L30 KUMAR049F/A
L31 STR L28
L32 2 S L31 CSS SAM SUB=L13
L33 17 S L31 CSS FUL SUB=L13
    SAV L33 KUMAR049G/A
L34 44 S L27,L30,L33
L35 41 S L34 NOT COMPD

```

FILE 'HCAOLD' ENTERED AT 14:56:54 ON 14 FEB 2003

```

L36 2 S L35
    SEL AN
    EDIT /AN /OREF

```

FILE 'HCAPLUS' ENTERED AT 14:57:17 ON 14 FEB 2003

L37 4 S E1-E2
L38 2 S L37 NOT (STOFFEL ? OR COLEBOURNE ?)/AU
L39 58 S L35
L40 1 S L39 AND (MAGDOLEN ? OR MORODER L? OR MOERODER ? OR MOROEDER ?
L41 0 S L39 AND WILEX?/PA,CS
L42 2 S L38 AND L39
L43 3 S L40,L42
L44 56 S L39 AND (PD<20000823 OR PRD<=20000823 OR AD<=20000823)
L45 47 S L44 AND P/DT
L46 16 S L45 AND US/PC
L47 18 S L43,L46

FILE 'REGISTRY' ENTERED AT 15:03:06 ON 14 FEB 2003

L48 STR
L49 0 S L48 CSS SAM
L50 STR L48
L51 0 S L50 CSS
L52 0 S L50 SAM
L53 30 S L50 FUL
SAV L53 KUMAR049H/A
L54 24 S L53 NOT SQL/FA
L55 1 S L54 AND C10H14N8S4

FILE 'HCAOLD' ENTERED AT 15:11:46 ON 14 FEB 2003

L56 0 S L55

FILE 'HCAPLUS' ENTERED AT 15:11:49 ON 14 FEB 2003

L57 1 S L55
L58 19 S L47,L57

FILE 'REGISTRY' ENTERED AT 15:12:25 ON 14 FEB 2003

L59 1 S UROKINASE PLASMINOGEN ACTIVATOR/CN

FILE 'HCAPLUS' ENTERED AT 15:12:27 ON 14 FEB 2003

L60 0 S L59 AND L58
L61 0 S L59 AND L39

FILE 'REGISTRY' ENTERED AT 15:12:59 ON 14 FEB 2003

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 15:13:48 ON 14 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 14 Feb 2003 VOL 138 ISS 8

FILE LAST UPDATED: 13 Feb 2003 (20030213/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 158 all hitstr tot

L58 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:730738 HCAPLUS

DN 135:288789

TI 2-Substituted 4-heteroaryl-pyrimidines with activity as inhibitors of cyclin-dependent kinases and their preparation and use in the treatment of proliferative disorders

IN Fischer, Peter Martin; Wang, Shudong

PA Cyclacel Limited, UK

SO PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D409-04

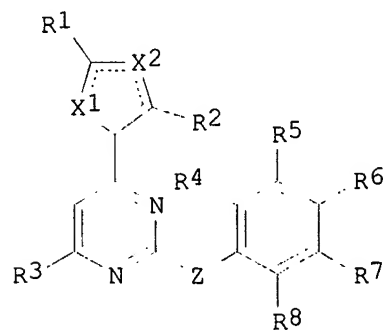
ICS C07D417-04; C07D417-14; A61K031-506; A61P035-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

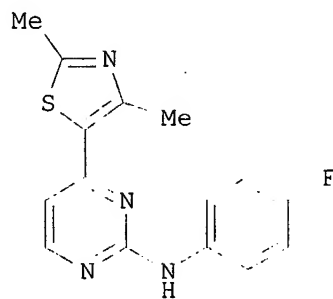
Section cross-reference(s): 1, 7

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2001072745	A1	20011004	WO 2001-GB1423	20010328	<--
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	GB 2361236	A1	20011017	GB 2001-7758	20010328	<--
	GB 2361236	B2	20020424			
	EP 1274705	A1	20030115	EP 2001-915544	20010328	<--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2002019404	A1	20020214	US 2001-823075	20010329	<--
PRAI	GB 2000-7636	A	20000329			<--
	GB 2000-15117	A	20000620			<--
	WO 2001-GB1423	W	20010328			
OS	MARPAT 135:288789					
GI						



I



IV

AB The invention relates to 2-substituted 4-heteroaryl-pyrimidines I and their pharmaceutically acceptable salts [wherein: X1 = CH and X2 = S; or 1 of X1 and X2 = S and the other = N; Z = NH, NHCO, NHSO2, NHCH2, CH2, CH2CH2, or CH:CH; R1, R2, R3 = H, alkyl, aryl, aralkyl, heterocyclyl,

halo, NO₂, cyano, OH, alkoxy, aryloxy, NH₂, NHR', N(R')(R''), NHCOR', NH(aryl), N(aryl)₂, COOH, COOR', COO(aryl), CONH₂, CONHR', CON(R')(R''), CONH(aryl), CON(aryl)₂, SO₃H, SO₂NH₂, CF₃, COR', or CO(aryl), wherein alkyl, aryl, aralkyl, heterocyclyl, and NH(aryl) groups may be further substituted with 1 or more halo, NO₂, cyano, OH, OMe, NH₂, COOH, CONH₂, and/or CF₃; at least 1 of R₁ and R₂ .noteq. H when either X₁ or X₂ = S; R₄, R₅, R₆, R₇, R₈ = H, (un)substituted alkyl, halo, NO₂, cyano, OH, (un)substituted alkoxy, NH₂, NHR', alkyl-aryl, alkyl-heteroaryl, NH(C:NH)NH₂, N(R')₃⁺, N(R')(R''), COOH, COOR', CONH₂, CONHR', CON(R')(R''), SO₃H, SO₂NH₂, CF₃, or (CH₂)_nO(CH₂)_mNR'R'', (CH₂)_nCO₂(CH₂)_mOR''' wherein n = 0, 1, 2, or 3; m = 1, 2 or 3; R', R'', R''' = alkyl]. The invention also relates to prepn. of I, pharmaceutical compns. contg. them, and their use as inhibitors of cyclin-dependant kinases (CDKs), and hence their use in the treatment of proliferative disorders such as cancer, leukemia, psoriasis and the like. Examples include 22 syntheses and a variety of bioassays. For instance, 4-FC6H₄NH₂ was treated with HNO₃ and cyanamide in EtOH to give 47% 4-FC6H₄NHC(:NH)NH₂.HNO₃ (II). Sep., 5-acetyl-2,4-dimethylthiazole was condensed with N,N-dimethylformamide di-Me acetal to give 79% 3-dimethylamino-1-(2,4-dimethylthiazol-5-yl)propenone (III). Cyclocondensation of II with III in refluxing MeOCH₂CH₂OH in the presence of NaOH gave title compd. IV in 89% yield. In an assay against multiple kinases, IV selectively inhibited CDKs, showing an IC₅₀ of 0.019 .mu.M against CDK2/cyclin E, and 0.47 .mu.M against CDK4/cyclin D1, vs. >20 .mu.M against PCK.alpha. and SAPK2a. Addnl. bioassays of I showed antiproliferative and cytotoxic activity.

- ST heteroarylpyrimidine prepn antiproliferative anticancer cytotoxic; pyrimidine thiazolyl thienyl prepn inhibitor CDK; kinase cyclin dependent inhibitor heteroarylpyrimidine prepn
- IT Antitumor agents
(leukemia; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)
- IT Antitumor agents
(prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)
- IT Proliferation inhibition
(proliferation inhibitors; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)
- IT 90698-26-3, S6 kinase 137632-08-7, ERK-2 kinase 165245-96-5, Stress-activated protein kinase-2a
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(comparative inhibition; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)
- IT 364333-82-4P 364334-16-7P 364334-85-0P 364334-88-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)
- IT 364333-71-1P 364333-72-2P 364333-73-3P 364333-74-4P 364333-75-5P
364333-76-6P 364333-77-7P 364333-78-8P 364333-79-9P 364333-80-2P
364333-81-3P 364333-83-5P 364333-84-6P 364333-85-7P 364333-86-8P
364333-88-0P 364333-89-1P 364333-90-4P 364333-91-5P 364333-92-6P
364333-93-7P 364333-94-8P 364333-95-9P 364333-96-0P 364333-97-1P
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364334-29-2P 364334-30-5P 364334-31-6P 364334-32-7P 364334-33-8P

364334-34-9P 364334-35-0P 364334-36-1P 364334-37-2P 364334-38-3P
 364334-39-4P 364334-40-7P 364334-41-8P 364334-42-9P 364334-43-0P
 364334-44-1P 364334-45-2P 364334-46-3P 364334-47-4P 364334-48-5P
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 364334-64-5P 364334-66-7P 364334-67-8P 364334-68-9P 364334-69-0P
 364334-70-3P 364334-71-4P 364334-72-5P 364334-73-6P 364334-74-7P
 364334-75-8P 364334-76-9P 364334-77-0P 364334-78-1P 364334-79-2P
 364334-80-5P 364334-81-6P 364334-82-7P 364334-83-8P 364334-84-9P
 364334-86-1P 364334-87-2P 364334-89-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

IT 141349-86-2, CDK2 kinase 144378-32-5, Cyclin B-Cdk1 kinase
 146279-89-2, Cyclin E-Cdk2 kinase 147014-97-9, CDK4 kinase 150428-23-2
 166433-53-0, Cyclin D1-Cdk4 kinase

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(inhibitors; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

IT 27692-74-6P 38647-83-5P 65783-22-4P 71198-32-8P 72833-78-4P
 122229-18-9P 142992-99-2P 364334-90-7P 364334-91-8P 364334-93-0P
 364334-94-1P 364334-95-2P 364334-96-3P 364334-98-5P 364335-05-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

IT 99-09-2, 3-Nitroaniline 106-47-8, 4-Chloroaniline, reactions 113-00-8, Guanidine 119-34-6, 4-Amino-2-nitrophenol 121-51-7, 3-Nitrobenzenesulfonyl chloride 367-25-9, 2,4-Difluoroaniline 371-40-4, 4-Fluoroaniline 420-04-2, Cyanamide 455-19-6 598-52-7 869-24-9 1083-48-3, 4-(4-Nitrobenzyl)pyridine 1694-29-7, 3-Chloro-2,4-pentadione 2530-10-1, 3-Acetyl-2,5-dimethylthiophene 4621-66-3, Thionicotinamide 4637-24-5 7660-21-1 38205-60-6, 5-Acetyl-2,4-dimethylthiazole 67453-82-1 100224-74-6, Guanidine carbonate 166196-79-8 314268-62-7 364335-00-2 364335-01-3 364335-02-4 364335-03-5 **364335-04-6**

RL: RCT (Reactant); RACT (Reactant or reagent)

(precursor; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

IT 141436-78-4

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(.alpha., comparative inhibition; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Breault, G; WO 0012485 A 2000 HCAPLUS
- (2) Celltech Therapeutics Ltd; WO 9719065 A 1997 HCAPLUS
- (3) Ciba Geigy Ag; WO 9509847 A 1995 HCAPLUS
- (4) Zimmermann, J; ARCHIV DER PHARMAZIE 1996, V329(7), P371 HCAPLUS

IT **364335-04-6**

RL: RCT (Reactant); RACT (Reactant or reagent)

(precursor; prepn. of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

RN 364335-04-6 HCAPLUS

CN Guanidine, [4-(hydroxymethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L58 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:96024 HCAPLUS

DN 132:137409

TI Preparation of tryptase inhibitors

IN Rice, Ken Duane; Dener, Jeffrey Mark; Gangloff, Anthony Robert; Kuo, Elaine Yee-lin

PA AXYS Pharmaceuticals, Inc., USA

SO U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 312,269, abandoned.

CODEN: USXXAM

DT **Patent**

LA English

IC ICM C07D295-32

ICS C07D295-205

NCL 544357000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6022969	A	20000208	US 1995-522157	19950914 <--
	CA 2200561	AA	19960328	CA 1995-2200561	19950914 <--
	CN 1160398	A	19970924	CN 1995-195191	19950914 <--
	HU 77770	A2	19980828	HU 1997-2059	19950914 <--
	ZA 9508028	A	19960418	ZA 1995-8028	19950922 <--
	TW 442478	B	20010623	TW 1995-84110031	19950926 <--
	LT 4234	B	19971027	LT 1997-65	19970410 <--
	LV 11865	B	19980120	LV 1997-70	19970422 <--
	US 6211228	B1	20010403	US 1999-280227	19990329 <--
PRAI	US 1994-312269	B2	19940923	<--	
	US 1995-522157	A3	19950914	<--	

OS MARPAT 132:137409

AB (ZX1X2X3X4X5)2Y [X1 = (oxa)alkylene, phenylene-interrupted alkylene, etc.; X2,X4 = CO, CO₂, OCO₂, CONH, etc.; X3 = alkylene, X9X10, X10X9, etc.; X5,X9 = alkylene; X10,Y = (hetero)cycloalkylene; Z = NH₂, NHC(:NH)NH₂, C(:NH)NH₂] were prepd. Thus, trans-cyclohexanedimethanol was bisesterified by OCNCH₂CO₂Et and the sapond. product bisamidated by 4-(H₂N)C₆H₄CH₂NH₂ to give, after NCNH₂ N-acylation, Y[CH₂O₂CNHCH₂CONHCH₂C₆H₄[NHC(:NH)NH₂]-4]2 (Y = trans-1,4-cyclohexylene). Data for biol. activity of title inhibitors were given.

ST tryptase inhibitor prepn

IT Antiasthmatics

(prepn. of tryptase inhibitors)

IT 97501-93-4, Tryptase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(mediated disorders; treatment; prepn. of tryptase inhibitors)

IT	178972-17-3P	178972-18-4P	178972-19-5P	178972-43-5P	178972-44-6P
	178972-45-7P	178972-46-8P	178972-49-1P	178972-51-5P	178972-52-6P
	178972-55-9P	178972-56-0P	178972-59-3P	178972-60-6P	178972-61-7P
	178972-62-8P	178972-63-9P	178972-66-2P	178972-67-3P	178972-68-4P
	178972-69-5P	178972-70-8P	178972-71-9P	178972-72-0P	178972-74-2P

178972-75-3P 178972-77-5P 178972-78-6P 178972-79-7P 178972-80-0P
178972-81-1P 178972-83-3P 178972-84-4P 178972-85-5P 178972-86-6P
178972-87-7P 178972-88-8P 178972-90-2P 178972-91-3P 178972-92-4P
256649-14-6P 256649-19-1P 256649-21-5P 256649-27-1P 256649-29-3P
256649-31-7P 256649-32-8P 256649-33-9P 256649-34-0P 256649-36-2P
256649-37-3P 256649-38-4P 256649-39-5P 256649-40-8P 256649-41-9P
256649-42-0P 256649-43-1P 256649-52-2P 256649-55-5P 256649-60-2P
257296-41-6P 257296-42-7P 257296-43-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tryptase inhibitors)

IT 1197-18-8, trans-4-Aminomethylcyclohexanecarboxylic acid 2949-22-6,
Ethyl isocyanatoacetate 3236-48-4, trans-1,4-Cyclohexanedimethanol
4403-71-8, 4-Aminobenzylamine 23418-82-8, cis-1,5-Cyclooctanediol
57260-71-6, tert-Butyl 1-piperazinecarboxylate 76197-74-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of tryptase inhibitors)

IT 59878-28-3P 172348-63-9P 174959-54-7P **174959-57-0P**
178972-20-8P 178972-21-9P 178972-23-1P 178972-25-3P 178972-28-6P
178972-29-7P 178972-30-0P 178972-32-2P 178972-33-3P 178972-34-4P
178972-35-5P 178972-36-6P 178972-37-7P 178972-38-8P 178972-39-9P
178972-40-2P 178972-41-3P 192323-08-3P 202979-19-9P 202979-20-2P
256649-56-6P 256649-57-7P 256649-58-8P 256649-59-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of tryptase inhibitors)

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; EP 214429 1987 HCAPLUS
- (2) Anon; WO 9420527 1994 HCAPLUS
- (3) Anon; WO 9532945 1995 HCAPLUS
- (4) Castells; J Allergy Clin Immunol 1988, V82, P348 MEDLINE
- (5) Caughey; Am J Respir Cell Mol Biol 1991, V4, P387 HCAPLUS
- (6) Caughey; J Pharmacol Exp Ther 1988, V244, P133 HCAPLUS
- (7) Chiu; Arch, Int, Pharmacodyn 1984, V270, P128 HCAPLUS
- (8) Cotrel; US 4220646 1980 HCAPLUS
- (9) Franconi; J Pharmacol Exp Ther 1988, V248(3), P947
- (10) Fujii; US 4746737 1988 HCAPLUS
- (11) Kalenderian; Chest 1988, V94, P119 MEDLINE
- (12) Larsen; The Lung:Scientific Foundations 1991, P953
- (13) Lum; US 5656660 1997 HCAPLUS
- (14) Miller; J Clin, Invest 1989, V84, P1188 HCAPLUS
- (15) Miller; J Clin, Invest 1990, V86, P864 HCAPLUS
- (16) Ruoss; J Clin, Invest 1991, V88, P493 HCAPLUS
- (17) Schwartz; N Engl J Med 1987, V316, P1622 MEDLINE
- (18) Sekizawa; J Clin, Invest 1989, V83, P175 HCAPLUS
- (19) Spear; US 5525623 1996 HCAPLUS
- (20) Sturzebecher; Biol Chem Hoppe-Seyler 1992, V373, P1025 MEDLINE
- (21) Tam; Am J Respir, Cell Mol Biol 1990, V3, P27 HCAPLUS
- (22) Tidwell; Antimicrobial Agents and Chemotherapy 1984, V26, P591 HCAPLUS
- (23) Tidwell; J Med Chem 1983, V26, P294 HCAPLUS
- (24) Vanderslice; Biochemistry 1989, V28, P4148 HCAPLUS
- (25) Vanderslice; Proc Natl Acad, Sci USA 1990, V87, P3811 HCAPLUS
- (26) Wanner; Am Rev Respir, Dis 1990, V141, P253 MEDLINE
- (27) Wenzel; Am Rev Resp Dis 1988, V141, P1002

IT **174959-57-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of tryptase inhibitors)

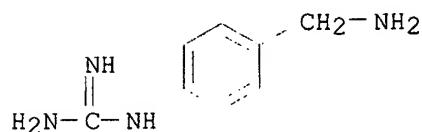
RN 174959-57-0 HCAPLUS

CN Guanidine, [4-(aminomethyl)phenyl]-, bis(trifluoroacetate) (9CI) (CA
INDEX NAME)

CM 1

CRN 174959-56-9

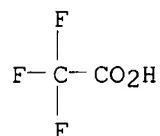
CMF C8 H12 N4



CM 2

CRN 76-05-1

CMF C2 H F3 O2



L58 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1999:708594 HCAPLUS

DN 131:310457

TI Preparation of aryl-substituted guanidines for treating mitochondria-associated diseases

IN Ghosh, Soumitra; Davis, Robert E.

PA Mitokor, USA

SO PCT Int. Appl., 61 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K031-155

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

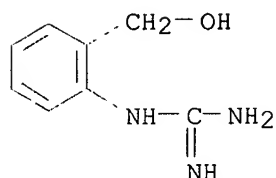
Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9955321	A1	19991104	WO 1999-US8880	19990423 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2329709	AA	19991104	CA 1999-2329709	19990423 <--
AU 9939656	A1	19991116	AU 1999-39656	19990423 <--
EP 1071414	A1	20010131	EP 1999-922721	19990423 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6268398	B1	20010731	US 1999-299044	19990423 <--
JP 2002512954	T2	20020508	JP 2000-545520	19990423 <--

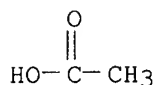
US 2002052409 A1 20020502 US 2001-875450 20010605 <--
 PRAI US 1998-82998P P 19980424 <--
 US 1999-299044 A1 19990423 <--
 WO 1999-US8880 W 19990423 <--
 OS MARPAT 131:310457
 AB The title compds. ArLNHC(:NH)NH2 [I; Ar = (un)substituted Ph or naphthyl;
 L = optional linker selected from (CH2)n, (CH2)nNH, etc.], useful for
 treating mitochondria-assocd. diseases, such as cancer, psoriasis, stroke,
 Alzheimer's disease and diabetes, were prepd. E.g., 4-
 HOC6H4CH2CH2NHC(:NH)NH2 was prepd. E.g., effect of I on ionomycin-induced
 apoptosis in cybrid cells was investigated.
 ST aryl substituted guanidine prepn mitochondria assocd disease
 IT Mitochondria
 (diseases; prepn. of aryl-substituted guanidines for treating
 mitochondria-assocd. diseases)
 IT Apoptosis
 (prepn. of aryl-substituted guanidines and their effect on apoptosis)
 IT 55-57-2P 2002-16-6P 13764-61-9P 22817-15-8P 26476-35-7P
 41610-50-8P 57004-63-4P 82957-07-1P 247234-16-8P 247234-17-9P
 247234-18-0P 247234-19-1P 247234-20-4P 247234-22-6P 247234-24-8P
 247234-25-9P 247234-26-0P 247234-27-1P 247234-29-3P 247234-30-6P
 247234-31-7P **247234-33-9P** 247234-35-1P 247234-37-3P
 247234-38-4P 247234-39-5P 247234-40-8P 247234-42-0P 247234-43-1P
 247234-44-2P 247234-46-4P 247234-47-5P 247234-49-7P 247234-50-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of aryl-substituted guanidines for treating
 mitochondria-assocd. diseases)
 IT 51-67-2 1620-98-0 2298-07-9 4023-02-3 107819-90-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aryl-substituted guanidines for treating
 mitochondria-assocd. diseases)
 IT 247234-51-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of aryl-substituted guanidines for treating
 mitochondria-assocd. diseases)
 RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
 (1) Childrens Hosp Medical Center; WO 9745108 A 1997 HCAPLUS
 (2) Dabrowski, A; J Physiol Pharmacol 1994, V45(3), P455
 (3) Hirano, T; Journal of International Medical Research 1992, V20(3), P211
 HCAPLUS
 (4) Luft, R; Proceedings of the National Academy of Sciences of USA 1994,
 V91(19), P8731 HCAPLUS
 (5) Marshall, F; US 3541218 A 1970 HCAPLUS
 (6) Medgene Limited; WO 9713504 A 1997 HCAPLUS
 (7) Michel, R; Biochem Pharmacol 1971, V20(10), P2587 HCAPLUS
 (8) Tanabe Seiyaku Co; EP 0790240 A 1997 HCAPLUS
 (9) Univ Strathclyde; WO 9636325 A 1996 HCAPLUS
 (10) Upjohn Co; WO 9303714 A 1993 HCAPLUS
 IT **247234-33-9P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of aryl-substituted guanidines for treating
 mitochondria-assocd. diseases)
 RN 247234-33-9 HCAPLUS
 CN Guanidine, [2-(hydroxymethyl)phenyl]-, monoacetate (salt) (9CI) (CA INDEX
 NAME)

CRN 247234-32-8
CMF C8 H11 N3 O



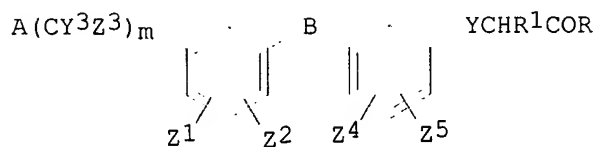
CM 2

CRN 64-19-7
CMF C2 H4 O2



L58 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2003 ACS
AN 1998:430106 HCAPLUS
DN 129:108912
TI Preparation of 3-guanidinophenylamides and related compounds as integrin .alpha.v.beta.3 inhibitors or antagonists.
IN Chandrakumar, Nizal; Chen, Barbara B.; Chen, Helen Y.; Clare, Michael; Gasiecki, Alan F.; Haack, Richard A.; Malecha, James W.; Ruminski, Peter G.; Russell, Mark A.
PA G. D. Searle & Co., USA
SO U.S., 77 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07C241-00
ICS C07C321-00; C07C205-00; C07C229-00
NCL 562439000
CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 28
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5773646	A	19980630	US 1997-825086	19970327 <--
PRAI	US 1997-825086		19970327		
OS	MARPAT 129:108912				
GI					



AB Title compds. [I; A = NR⁵C(Y¹)NR⁷R⁸, etc.; Y¹ = NR², O, S; R² = H, alkyl, aryl, OH, alkoxy, cyano, NO₂, amino, aminocarbonyl, alkenyl, alkynyl,

(substituted) alkyl, aryl, heterocyclyl; R2R7 = (substituted) heterocyclyl; R7, R8 = H, alkyl, alkenyl, alkynyl, aralkyl, cycloalkyl, bicycloalkyl, aryl, acyl, benzoyl, (substituted) alkyl, heterocyclyl, etc.; NR7R8 = (substituted) mono- or bicyclic heterocyclyl; R5 = H, alkyl, alkenyl, alkynyl, PhCH2, PhCH2CH2; Z1, Z2, Z4, Z5 = H, alkyl, OH, alkoxy, aryloxy, aralkoxy, halo, haloalkyl, haloalkoxy, NO2, amino, aminoalkyl, alkylamino, dialkylamino, cyano, alkylthio, alkylsulfonyl, carboxyl derivs., (fused) aryl; cycloalkyl, (fused) heterocyclyl, A; B = SO2NR50, CONR50(CH2)p, CH2O, SOCH2, SO2CH2, etc.; p = 0-2; R50 = H, alkyl; Y = (CHR70)q, 0; q = 0, 1; R70 = H, alkyl, (substituted) aryl; m = 0-2; R = XR3; X = O, S, NR4; R3, R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, aryl, aralkyl, etc.; Y3, Z3 = H, alkyl, aryl, cycloalkyl, aralkyl; R1 = H, alkyl, aryl, etc.], were prepd. Thus, 3-[[[3-[(aminomiminoethyl)amino]phenyl]sulfonyl]amino]-.beta.-phenylbenzenepropanoic acid trifluoroacetate (prepn. given) inhibited vitronectin adhesion with IC50 = 16.7 nM.

ST guanidinophenylamide prepn integrin inhibitor; anticancer
guanidinophenylamide

IT Antitumor agents

(metastasis; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT Angiogenesis inhibitors

Antitumor agents

(prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT Artery, disease

(restenosis, inhibitors; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT Muscle

(smooth, inhibitors of smooth muscle cell migration; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT Osteoporosis

(therapeutic agents; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT Integrins

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(.alpha.v.beta.3, inhibitors; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT 7440-70-2, Calcium, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (hypercalcemia; inhibitors; prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT	197790-15-1P	197790-17-3P	197790-18-4P	197790-19-5P	197790-20-8P
	197790-24-2P	197790-25-3P	197790-26-4P	197790-32-2P	197790-33-3P
	197790-34-4P	197790-35-5P	197790-36-6P	197790-38-8P	197790-39-9P
	197790-42-4P	197790-43-5P	197790-44-6P	197790-45-7P	197790-49-1P
	197790-51-5P	197790-52-6P	197790-53-7P	197790-54-8P	197790-55-9P
	197790-56-0P	197790-57-1P	197790-58-2P	197790-61-7P	197790-63-9P
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	197790-72-0P	197790-73-1P	197790-75-3P	197790-77-5P	197790-79-7P
	197790-81-1P	197790-83-3P	197790-84-4P	197790-85-5P	197790-87-7P
	197790-88-8P	197790-90-2P	197790-91-3P	197790-93-5P	197790-94-6P
	197790-95-7P	197790-96-8P	197790-97-9P	197790-98-0P	197790-99-1P
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	197791-38-1P	197791-39-2P	197791-40-5P	197791-42-7P	197791-44-9P
	197791-46-1P	197791-48-3P	197791-50-7P	197791-52-9P	197791-54-1P
	197791-55-2P	197791-57-4P	197791-59-6P	197791-61-0P	197791-63-2P

197791-65-4P	197791-67-6P	197791-69-8P	197791-71-2P	197791-74-5P
197791-75-6P	197791-77-8P	197791-80-3P	197791-83-6P	197791-85-8P
197791-87-0P	197791-96-1P	197792-24-8P	209916-37-0P	209916-38-1P
209916-39-2P	209916-40-5P	209916-41-6P	209916-42-7P	209916-43-8P
209916-44-9P	209916-45-0P	209916-46-1P	209916-47-2P	209916-48-3P
209916-49-4P	209916-50-7P	209916-51-8P	209916-52-9P	209916-53-0P
209916-55-2P	209916-56-3P	209916-57-4P	209916-58-5P	209916-59-6P
209916-60-9P	209916-61-0P	209916-62-1P	209916-63-2P	209916-64-3P
209916-65-4P	209916-66-5P	209916-67-6P	209916-68-7P	209916-69-8P
209916-70-1P	209916-71-2P	209916-72-3P	209916-73-4P	209916-74-5P
209916-75-6P	209916-76-7P	209916-77-8P	209916-78-9P	209916-79-0P
209916-80-3P	209916-81-4P	209916-82-5P	209916-83-6P	209916-84-7P
209916-85-8P	209916-86-9P	209916-87-0P	209916-88-1P	209916-89-2P
209916-90-5P	209916-91-6P	209916-92-7P	209916-93-8P	209916-94-9P
209916-95-0P	209916-96-1P	209916-97-2P	209916-98-3P	209916-99-4P
209917-00-0P	209917-02-2P			

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT 79-03-8, Propionyl chloride 95-56-7, 2-Bromophenol 99-05-8 99-61-6
 100-58-3, Phenylmagnesium bromide 109-76-2, 1,3-Propanediamine
 121-51-7 121-71-1 121-90-4 121-92-6 135-02-4, o-Anisaldehyde
 141-82-2, Propanedioic acid, reactions 311-46-6, Ethyl
 dimethylphosphonoacetate 403-43-0, 4-Fluorobenzoyl chloride 532-55-8,
 Benzoyl isothiocyanate 543-24-8, N-Acetylglycine 582-33-2, Ethyl
 3-aminobenzoate 585-79-5 586-39-0, 3-Nitrostyrene 591-27-5,
 3-Aminophenol 621-36-3 622-78-6, Benzyl isothiocyanate 867-13-0
 1016-77-9, 3-Bromobenzophenone 1066-54-2 1877-72-1 1878-67-7,
 3-Bromophenylacetic acid 2525-16-8 2719-30-4, 2-Nitrophenyl
 isothiocyanate 2840-28-0, 3-Amino-4-chlorobenzoic acid 2905-62-6,
 3,5-Dichlorobenzoyl chloride 3173-56-6 3320-87-4, 3-Nitrophenyl
 isocyanate 3485-84-5, N-Vinylphthalimide 3943-95-1, Methyl
 3-hydroxycinnamate 3958-57-4 4518-10-9, Methyl 3-aminobenzoate
 5292-43-3, tert-Butyl bromoacetate 6136-68-1, 3-Acetylbenzonitrile
 10203-08-4, 3,5-Dichlorobenzaldehyde 13020-57-0, 3-Hydroxybenzophenone
 14338-36-4, 3-Aminophenylacetic acid 22948-02-3, 3-Mercaptoaniline
 24964-64-5 37182-75-5 39959-54-1, 3-Bromobenzylamine hydrochloride
 62327-21-3 90567-37-6 129714-97-2, 3,5-Difluorobenzoyl chloride
 135007-62-4 173300-83-9 174484-84-5 177787-26-7,
 3,4,5-Trifluorobenzoyl chloride 197792-81-7 197792-91-9 197792-95-3
 197793-32-1 197793-34-3 197793-35-4 197793-62-7 197793-78-5,
 5-Methoxy-2-nitrophenyl isothiocyanate 209917-45-3 209917-47-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

IT 555-68-0P 1197-05-3P 1664-54-6P 6136-62-5P 13428-06-3P
 32858-79-0P 33877-05-3P 36412-61-0P 40872-87-5P 42823-33-6P
 50916-34-2P 52797-97-4P 55197-35-8P 69355-34-6P 79119-25-8P
 90418-21-6P 103860-22-6P 104508-22-7P 115750-83-9P 118647-53-3P
 132691-37-3P 135482-72-3P 163978-50-5P 171663-13-1P 178445-92-6P
 188812-06-8P 188812-08-0P 188812-11-5P 188812-92-2P 188812-93-3P
 188813-00-5P 197719-68-9P 197791-99-4P 197792-00-0P 197792-01-1P
 197792-02-2P 197792-03-3P 197792-04-4P 197792-05-5P 197792-06-6P
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 197792-53-3P 197792-54-4P 197792-55-5P 197792-57-7P
 197792-59-9P 197792-60-2P 197792-61-3P 197792-62-4P
 197792-63-5P 197792-64-6P 197792-65-7P 197792-66-8P 197792-67-9P

197792-68-0P	197792-69-1P	197792-70-4P	197792-72-6P	197792-73-7P
197792-82-8P	197792-85-1P	197792-93-1P	197792-94-2P	197792-96-4P
197792-97-5P	197792-98-6P	197792-99-7P	197793-00-3P	197793-01-4P
197793-03-6P	197793-04-7P	197793-05-8P	197793-06-9P	197793-07-0P
197793-08-1P	197793-09-2P	197793-10-5P	197793-11-6P	197793-12-7P
197793-13-8P	197793-14-9P	197793-15-0P	197793-17-2P	197793-18-3P
197793-19-4P	197793-20-7P	197793-21-8P	197793-22-9P	197793-24-1P
197793-25-2P	197793-26-3P	197793-28-5P	197793-30-9P	197793-37-6P
197793-38-7P	197793-39-8P	197793-40-1P	197793-41-2P	197793-43-4P
197793-46-7P	197793-48-9P	197793-51-4P	197793-53-6P	197793-56-9P
197793-64-9P	197793-65-0P	197793-68-3P	209917-21-5P	209917-23-7P
209917-30-6P	209917-31-7P	209917-32-8P	209917-34-0P	209917-41-9P
209917-43-1P				

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anon; EP 0478328 A1 1992 HCAPLUS

(2) Anon; EP 0478363 A2 1992 HCAPLUS

(3) Anon; WO 9532710 1995 HCAPLUS

(4) Cain; US 5523302 1996 HCAPLUS

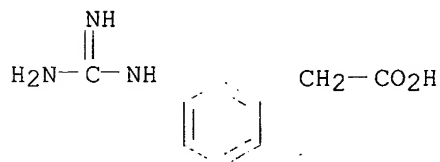
IT 197792-59-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 3-guanidinophenylamides and related compds. as integrin inhibitors or antagonists)

RN 197792-59-9 HCAPLUS

CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L58 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:430105 HCAPLUS

DN 129:95328

TI Preparation of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors

IN Chen, Barbara B.; Chen, Helen Y.; Clare, Michael; Rao, Shashidhar N.; Russell, Mark A.

PA G. D. Searle & Co., USA

SO U.S., 29 pp.

CODEN: USXXAM

DT Patent

LA English

IC ICM C07C241-00

ICS C07C229-00; C07D239-00

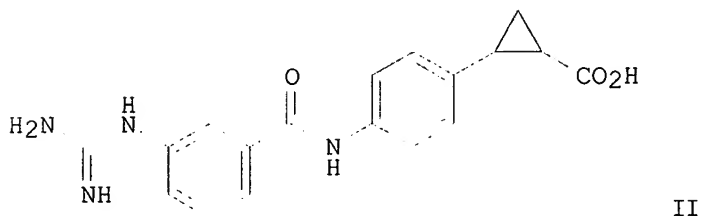
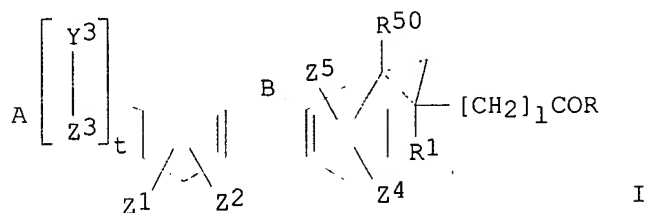
NCL 562439000

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5773644	A	19980630	US 1997-825040	19970327 <--
PRAI	US 1997-825040		19970327 <--		
OS	MARPAT 129:95328				
GI					



- AB Title compds. I [wherein Y1 = NR2, O, S; R2 = H, alkyl, aryl, etc.; R7, R8 = H, alkyl, alkenyl, etc.; R5 = H, alkyl, alkenyl, etc., NR5C(:NR7)Y2 (Y2 = alkyl, cycloalkyl, bicycloalkyl); Z1, Z2, Z4, Z5 = H, alkyl, OH, etc.; B = CH2CONH, C(O)O, SO2NH, etc.; l = 0-3; t = 0-2; R50 = H, alkyl, aryl; R = XR3 (wherein X = O, S, NR4; R3, R4 = H, alkyl, alkenyl); Y3, Z3 = H, alkyl, aryl, etc.; R1 = NHC(O)R12, NHC(O)OR12; NHSO2R12, etc. (wherein R12 = H, alkyl, cycloalkyl, etc.)] and their pharmaceutically acceptable salts are disclosed. The compds. are selective inhibitors or antagonists of .alpha.v.beta.3 integrin, and are thus useful for treating tumor metastasis, solid tumor growth, angiogenesis, osteoporosis, humoral hypercalcemia of malignancy, smooth muscle cell migration, and restenosis. Thus, 3-guanidinobenzoic acid.HCl was coupled with Et 2-(4-aminophenyl)cyclopropanecarboxylate using 1-methylpiperidine and iso-Bu chloroformate, and the ester product was partially hydrolyzed using LiOH in MeOH, to give after workup title compd. II.CF3COOH. In solid-phase receptor assays, the latter showed an IC50 value of 30.5 nM against .alpha.v.beta.3 integrin, but a less potent IC50 of 533 nM against IIb/IIIa receptors (indicator of undesired hematol. side effects).
- ST cyclopropanealkanoic acid prepn integrin antagonist inhibitor; antitumor agent cyclopropanealkanoic acid prepn; metastasis inhibitor cyclopropanealkanoic acid prepn; angiogenesis inhibitor cyclopropanealkanoic acid prepn; osteoporosis inhibitor cyclopropanealkanoic acid prepn; humoral hypercalcemia malignancy cyclopropanealkanoic acid prepn; smooth muscle cell migration cyclopropanealkanoate prepn; restenosis treatment cyclopropanealkanoic acid prepn
- IT Artery, disease
(coronary, restenosis, treatment of; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)
- IT Antitumor agents
(metastasis; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)
- IT Angiogenesis inhibitors

Antitumor agents
 (prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT Muscle, disease
 Muscle, disease
 (smooth, treatment of smooth muscle cell migration; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT Osteoporosis
 (therapeutic agents; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT Integrins
 RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
 (.alpha.v.beta.3; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT 7440-70-2, Calcium, biological studies
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (humoral hypercalcemia of malignancy; treatment of; prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT 198149-22-3P
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT 198149-21-2P 198149-23-4P 198149-24-5P 198149-26-7P 198149-27-8P
 198149-28-9P 198149-29-0P 198149-30-3P 198149-31-4P 198149-32-5P
 198149-33-6P 198149-34-7P 198149-35-8P 198149-36-9P 198149-37-0P
 198149-38-1P 198149-48-3P
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT 99-05-8, 3-Aminobenzoic acid 121-90-4, 3-Nitrobenzoyl chloride 367-24-8, 4-Bromo-2-fluoroaniline 503-87-7, 2-Thiohydantoin 582-33-2, Ethyl 3-aminobenzoate 1663-39-4, Tert-Butyl acrylate 2525-16-8, 1-Aza-2-methoxy-1-cycloheptene 4518-10-9, Methyl 3-aminobenzoate 5048-82-8, Ethyl 4-aminocinnamate 10191-60-3, Dimethyl N-cyanodithioiminocarbonate 14338-36-4, 3-Aminophenylacetic acid 24424-99-5, Di-tert-butyl dicarbonate 145013-05-4, N,N'-Bis(tert-butoxycarbonyl)thiourea
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

IT 42823-33-6P 90567-37-6P 93070-47-4P 144072-31-1P 183430-26-4P
 188812-06-8P 197719-68-9P 197792-59-9P 197792-93-1P
 197792-94-2P 198149-39-2P 198149-40-5P 198149-41-6P 198149-42-7P
 198149-43-8P 198149-44-9P 198149-45-0P 198149-46-1P 198149-47-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
 (1) Anon; EP 0478328 A1 1992 HCAPLUS
 (2) Anon; EP 0478363 A2 1992 HCAPLUS
 (3) Anon; WO 9532710 1995 HCAPLUS

(4) Cain; US 5523302 1996 HCAPLUS

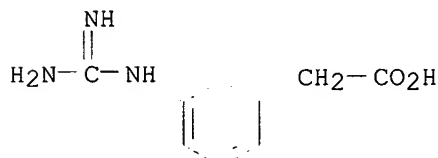
IT 197792-59-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenyl-substituted cyclopropanealkanoic acids as .alpha.v.beta.3 integrin antagonists or inhibitors)

RN 197792-59-9 HCAPLUS

CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L58 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1997:541857 HCAPLUS

DN 127:205895

TI Compositions and methods for treating mast-cell mediated conditions

IN Lum, Robert T.; Gschwend, Heinz W.; Bauer, Barr E.; Kuo, Elaine; Rice, Ken

PA Arris Pharmaceutical Corp., USA

SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 252,099.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-335

ICS A61K031-27; C07C271-06; C07C237-20

NCL 514467000

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5656660	A	19970812	US 1995-455286	19950531 <--
PRAI	US 1994-252099		19940601 <--		

OS MARPAT 127:205895

AB Comps. Z-(X1)n1-X2-X3-X4-(X5)n5-Y-(X'5)n'5-X'4-X'3-X'2-(X'1)n'1-Z' [Y = (un)substituted aryl; Z, Z' = aminomethyl- or guanyl-substituted Ph, cyclohexadienyl, cyclohexenyl, or cyclohexyl; X1, X'1, X5, X'5 = (un)substituted methylene; n1, n'1, n5, n'5 = 0 or 1; X2, X'2, X4, X'4 = NHCO, NHCONH, NHCO2, CONH, O2CNH or N-substituted derivs.; X3, X'3 = (un)substituted cycloalkylene, cycloheteroalkylene, alkylene] were prepd. for the treatment of mast cell mediated inflammatory conditions, such as conjunctivitis, asthma and allergic rhinitis. The comps. for treating mast cell mediated inflammatory conditions include oral, inhalant and topical preps. as well as devices comprising such preps. Thus, bis(p-xylylenediammoniumglycine)-1,4-benzenedimethanol dicarbamate bistrifluoroacetate was prepd. and assayed in vitro for inhibition of tryptase (Ki = 0.56 nM).

ST amino acid compd prepn inhibitor tryptase; mast cell tryptase inhibitor prepn

IT Nose

(allergic rhinitis; comps. and methods for treating mast-cell mediated

conditions)

IT Anti-inflammatory agents
Antiasthmatics
Mast cell
(compns. and methods for treating mast-cell mediated conditions)

IT 174958-67-9P 174958-68-0P 174958-69-1P 174958-70-4P 174958-72-6P
174958-73-7P 174958-74-8P 174958-75-9P 174958-76-0P 174958-77-1P
174958-79-3P 174958-80-6P 174958-81-7P 174958-82-8P 174958-84-0P
174958-85-1P 174958-86-2P 174958-87-3P 174958-88-4P 174958-89-5P
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174959-20-7P 174959-21-8P 174959-22-9P 174959-23-0P 174959-24-1P
174959-25-2P 174959-26-3P 174959-27-4P 174959-28-5P 174959-29-6P
174959-30-9P 174959-31-0P 174959-32-1P 174959-33-2P 174959-35-4P
174959-40-1P 174959-41-2P 174959-42-3P 174959-44-5P 174959-45-6P
174959-46-7P 174959-47-8P 174959-48-9P 175133-76-3P 175133-77-4P
194659-42-2P 194659-44-4P 194659-45-5P 194659-46-6P 194659-47-7P
194659-48-8P 194659-49-9P 194659-50-2P 194659-51-3P 194659-52-4P
194659-53-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(compns. and methods for treating mast-cell mediated conditions)

IT 97501-93-4, Tryptase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(compns. and methods for treating mast-cell mediated conditions)

IT 56-12-2, 4-Aminobutyric acid, reactions 56-40-6, Glycine, reactions
56-41-7, Alanine, reactions 56-91-7, 4-(Aminomethyl)benzoic acid
63-91-2, L-Phenylalanine, reactions 100-20-9, 1,4-Benzenedicarbonyl
dichloride 100-21-0, 1,4-Benzenedicarboxylic acid, reactions 105-10-2
105-53-3, Diethyl malonate 106-65-0 107-15-3, 1,2-Ethanediamine,
reactions 107-95-9, .beta.-Alanine 108-30-5, Succinic anhydride,
reactions 109-76-2, 1,3-Propanediamine 109-90-0, Ethyl isocyanate
110-60-1, 1,4-Butanediamine 147-85-3, Proline, reactions 338-69-2,
D-Alanine 420-04-2, Cyanamide 539-48-0, p-Xylylenediamine 589-29-7,
1,4-Benzenedimethanol 616-34-2, Glycine methyl ester 1013-88-3,
Benzophenone imine 1119-40-0 1119-48-8 1138-80-3 1197-18-8
1477-55-0, m-Xylylenediamine 1490-25-1, 3-Carbomethoxypropionyl chloride
1501-26-4, Methyl glutaryl chloride 4403-71-8, 4-Aminobenzylamine
5473-12-1, Sarcosine methyl ester 13093-02-2 20580-52-3 37031-29-1
37517-81-0, Methyl malonyl chloride 174959-86-5 174960-09-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(compns. and methods for treating mast-cell mediated conditions)

IT 5105-78-2P 10362-03-5P 27140-28-9P 27687-14-5P 31417-69-3P
33233-67-9P 57260-73-8P 68076-36-8P 75178-96-0P 98008-66-3P
108467-99-8P 108468-00-4P 111623-75-7P 174959-49-0P 174959-50-3P
174959-51-4P 174959-52-5P 174959-53-6P 174959-54-7P 174959-55-8P
174959-57-0P 174959-58-1P 174959-59-2P 174959-60-5P
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174959-96-7P 174959-97-8P 174959-98-9P 174960-04-4P 174960-05-5P
174960-06-6P 174960-07-7P 174960-08-8P 194659-54-6P 194659-55-7P
194659-56-8P 194659-58-0P 194659-59-1P 194659-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(compns. and methods for treating mast-cell mediated conditions)

IT **174959-57-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(comps. and methods for treating mast-cell mediated conditions)

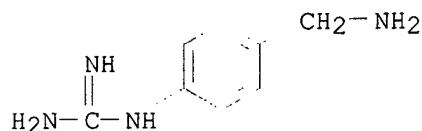
RN 174959-57-0 HCAPLUS

CN Guanidine, [4-(aminomethyl)phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 174959-56-9

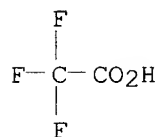
CMF C8 H12 N4



CM 2

CRN 76-05-1

CMF C2 H F3 O2



L58 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1996:209656 HCAPLUS

DN 124:261037

TI Preparation of 2-(pyridylmethylthio)benzimidazoles and analogs for control of Helicobacter bacteria

IN Hanauer, Guido; Simon, Wolfgang-Alexander; Zimmermann, Peter; Opferkuch, Wolfgang; Kohl, Bernhard; Grundler, Gerhard; Senn-Bilfinger, Joerg

PA Byk Gulden Lomberg Chemische Fabrik GmbH, Germany

SO PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DT **Patent**

LA German

IC ICM C07D401-12

ICS A61K031-44; C07D405-14; C07D417-14; C07D401-14; C07D471-04; C07D409-14

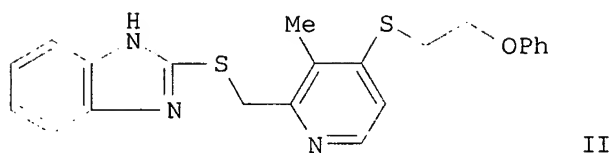
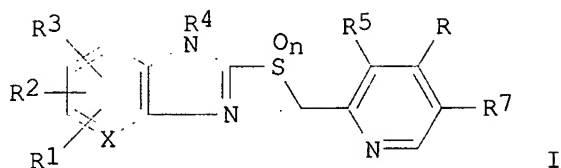
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9534554	A1	19951221	WO 1995-EP2237	19950609 <--
	W:	AU, BG, BY, CA, CN, CZ, EE, FI, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, UA, US			
	RW:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			
	CA 2192202	AA	19951221	CA 1995-2192202	19950609 <--
	AU 9527901	A1	19960105	AU 1995-27901	19950609 <--
	AU 697572	B2	19981008		
	EP 764161	A1	19970326	EP 1995-923288	19950609 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE			

HU 75516	A2	19970528	HU 1996-3339	19950609 <--
HU 220062	B	20011028		
CN 1159803	A	19970917	CN 1995-194562	19950609 <--
CN 1070488	B	20010905		
JP 10501254	T2	19980203	JP 1995-501598	19950609 <--
RU 2139286	C1	19991010	RU 1997-100641	19950609 <--
SK 281465	B6	20010409	SK 1996-1576	19950609 <--
CZ 288079	B6	20010411	CZ 1996-3624	19950609 <--
PL 181801	B1	20010928	PL 1995-317613	19950609 <--
RO 117792	B1	20020730	RO 1996-2255	19950609 <--
NO 9605162	A	19970205	NO 1996-5162	19961203 <--
FI 9604909	A	19961209	FI 1996-4909	19961209 <--
US 5859030	A	19990112	US 1997-750785	19970410 <--
PRAI CH 1994-1845	A	19940610 <--		
WO 1995-EP2237	W	19950609 <--		
OS MARPAT 124:261037				
GI				



AB Title compds. [I; R = SOpZ1(SOqZ2)mZ3Z4R6; R1 = H, halo, alkyl, alkoxy; R2 = H, halo, alkyl, alkoxy, etc.; R3 = H, (halo)alkoxy, OCClF2, etc.; R4 = H, alkyl, alkanoyl, etc.; R5 = H, alkyl, alkoxy; R6 = (di)alkylcarbonyl, N-alkyl-N'cyanoamidino, (hetero)aryl, etc.; X = CH or N; Z1, Z2 = alkylene; Z3 = O, SO0-2, (alkyl)imino; Z4 = bond, alkylene; n,p,q = 0 or 1] were prepd. Thus, 4-chloro-2,3-dimethylpyridine N-oxide was thioetherified by HSCH2CH2OH and the product treated with Ac2O to give, after chlorination, 4-(2-chloroethylthio)-2-chloromethyl-3-methylpyridine hydrochloride which was etherified by PhOH to give title compd. II. The latter had MIC 50 of 0.05.mu.g/mL against Helicobacter pylori.

ST pyridylmethylthiobenzimidazole prepn control Helicobacter

IT Bactericides, Disinfectants, and Antiseptics
Helicobacter

(prepn. of 2-(pyridylmethylthio)benzimidazoles and analogs for control of Helicobacter bacteria)

IT	162279-85-8P	175073-82-2P	175073-83-3P	175073-84-4P	175073-85-5P
	175073-86-6P	175073-87-7P	175073-88-8P	175073-89-9P	175073-90-2P
	175073-91-3P	175073-92-4P	175073-93-5P	175073-94-6P	175073-95-7P
	175073-96-8P	175073-97-9P	175073-98-0P	175073-99-1P	175074-00-7P
	175074-01-8P	175074-02-9P	175074-03-0P	175074-04-1P	175074-16-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 2-(pyridylmethylthio)benzimidazoles and analogs for control of Helicobacter bacteria)

IT 98-02-2, 2-Furanmethanethiol 108-95-2, Phenol, reactions 147-93-3,

2-Mercaptobenzoic acid 149-30-4, 2(3H)-Benzothiazolethione 583-39-1,
 2-Mercapto-1H-benzimidazole 1191-08-8, 1,4-Butanedithiol 1450-85-7,
 2-Mercaptopyrimidine 2382-96-9, 2-Mercaptobenzoxazole 4498-99-1,
 4-Methylbenzyl mercaptan 13182-81-5 13183-79-4 19721-22-3,
 3-Hydroxypropyl mercaptan 59886-85-0 59886-90-7, 4-Chloro-2,3-
 dimethylpyridine N-oxide 61607-68-9, 1-(2-Dimethylaminoethyl)-5-
 mercaptotetrazole 74470-32-9, Methyl 2-mercaptonicotinate 80646-14-6,
 5-Dimethylaminomethyl-2-furylmethylthiol **95853-51-3**,
 2-Guanidinothiazole-4-methylthiol 103949-59-3, 3,4-Dichloro-2-
 hydroxymethylpyridine 122307-41-9, 4-Chloro-3-methoxy-2-methylpyridine
 N-oxide 162280-00-4 175074-13-2 175074-14-3 175074-15-4
 175074-17-6, 2-(5-Methyl-4-thiazolyl)ethylthiol

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of 2-(pyridylmethylthio)benzimidazoles and analogs for control
 of Helicobacter bacteria)

IT 153284-81-2P 162279-97-2P 162279-99-4P 162280-03-7P 162280-06-0P
 162280-10-6P 170105-80-3P 170105-81-4P 175074-05-2P 175074-06-3P
 175074-07-4P 175074-08-5P 175074-09-6P 175074-10-9P 175074-11-0P
 175074-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of 2-(pyridylmethylthio)benzimidazoles and analogs for control
 of Helicobacter bacteria)

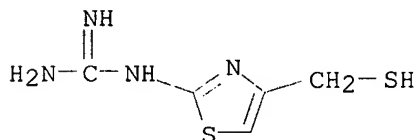
IT **95853-51-3**, 2-Guanidinothiazole-4-methylthiol

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of 2-(pyridylmethylthio)benzimidazoles and analogs for control
 of Helicobacter bacteria)

RN 95853-51-3 HCAPLUS

CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L58 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1992:214925 HCAPLUS

DN 116:214925

TI Preparation of (guanidinobenzoyl)di-peptides and related compounds as
 antithrombotics

IN Klein, Scott I.; Molino, Bruce F.

PA Rorer Pharmaceutical Corp., USA

SO U.S., 6 pp.

CODEN: USXXAM

DT **Patent**

LA English

IC A01K031-195; A01K031-415; A01K031-405; C07C279-00

NCL 514399000

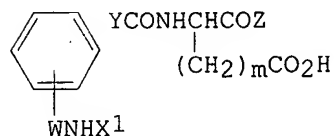
CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5086069	A	19920204	US 1990-475043	19900205 <--
	WO 9218117	A1	19921029	WO 1991-US2471	19910411 <--
	W: AU, CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	AU 9180896	A1	19921117	AU 1991-80896	19910411 <--
	AU 661659	B2	19950803		

EP 584066 A1 19940302 EP 1991-910671 19910411 <--
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
 JP 08503920 T2 19960430 JP 1991-510398 19910411 <--
 PRAI US 1990-475043 19900205 <--
 WO 1991-US2471 19910411 <--
 OS MARPAT 116:214925
 GI



AB Title compds. [I; Y = (CH₂)_n, CH:CH, XCH₂; X not defined; Z = NR₁R₂, OR₁; W = (CH₂)_n CH:CH(CH₂)_p; R₁, R₂ = alkyl, aryl, aralkyl, allyl; m = 1-3; n = 0-6; p = 0-4; X₁ = H, amidino], were prepd. Thus, L-valine p-alkoxybenzyl alc. resin ester was coupled with N-(9-fluorenylmethoxycarbonyl)aspartic acid .beta.-tert-Bu ester; the product was deprotected with piperidine in DMF followed by condensation with 3-(2-guanidinoethyl)benzoic acid hydrochloride (prepn. given) and resin cleavage with CF₃CO₂H to give N-(3-(2-guanidinoethyl)benzoyl)aspartylvaline. N-(3-Guanidinomethylbenzoyl)aspartylvaline, prepd. similarly, inhibited 125I-fibrinogen binding to platelets with IC₅₀ = 0.25 .mu.M.

ST guanidinobenzoyldipeptide prepn antithrombotic; dipeptide guanidinobenzoyl prepn antithrombotic; peptide guanidinobenzoyl prepn antithrombotic

IT Anticoagulants and Antithrombotics
 ((guanidinobenzoyl)dipeptides)

IT Peptides, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (di-, guanidinobenzoyl, prepn. of, as antithrombotics)

IT 141028-95-7P 141028-96-8P 141028-97-9P 141028-98-0P 141028-99-1P
 141029-00-7P 141029-01-8P 141029-02-9P 141029-03-0P 141029-04-1P
 141029-05-2P 141029-06-3P 141029-08-5P 141029-10-9P 141029-12-1P
 141029-14-3P 141029-15-4P 141029-16-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. of, as antithrombotic)

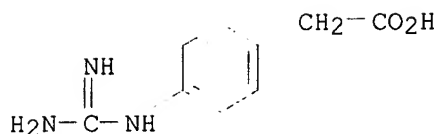
IT 25647-25-0P 42823-33-6P 42823-46-1P 52997-74-7P 81196-09-0P
 82957-07-1P, 3-Guanidinobenzoic acid 141029-17-6P 141029-18-7P
 141029-19-8P 141029-20-1P 141029-21-2P 141029-22-3P 141029-23-4P
141029-24-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for (guanidinobenzoyl)dipeptide antithrombotic)

IT 56-91-7, 4-Aminomethylbenzoic acid 99-05-8, 3-Aminobenzoic acid
 150-13-0, 4-Aminobenzoic acid 1184-90-3, Aminoiminomethanesulfonic acid
 2338-75-2, 4-Trifluoromethylphenylacetonitrile 2338-76-3,
 3-Trifluoromethylphenylacetonitrile 2393-20-6, 3-Aminomethylbenzoic acid
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in prepn. of (guanidinobenzoyl)dipeptide antithrombotic)

IT **141029-24-5P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for (guanidinobenzoyl)dipeptide antithrombotic)

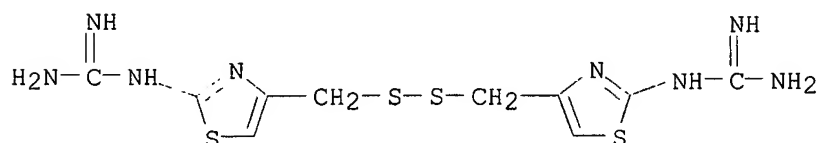
RN 141029-24-5 HCAPLUS

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, monohydrochloride (9CI)
 (CA INDEX NAME)



● HCl

L58 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1990:578363 HCAPLUS
 DN 113:178363
 TI Validation of a method for the assay of related compounds in famotidine raw materials and formulations
 AU Beaulieu, N.; Graham, S. J.; Sears, R. W.; Lovering, E. G.
 CS Bur. Drug Res., Health and Welfare Canada, Ottawa, ON, K1A 0L2, Can.
 SO Journal of Pharmaceutical and Biomedical Analysis (1989), 7(12), 1705-9
 CODEN: JPBADA; ISSN: 0731-7085
 DT Journal
 LA English
 CC 64-3 (Pharmaceutical Analysis)
 AB A HPLC method has been developed for the detn. of famotidine and related compds. in bulk and in formulations. The min. detectable amt. of the available related compds. was <0.02% and the min. quantifiable amt. <0.1%. Famotidine impurity levels were between 0.5 and 2.5% in bulk 0.44% in one tablet sample and about 3% in an i.v. soln.
 ST famotidine detn formulation HPLC; chromatog famotidine detn formulation; HPLC famotidine detn formulation
 IT 76823-93-3 76823-94-4 76824-14-1 76824-16-3 106433-44-7
 107880-74-0 109467-06-3 124646-10-2 **129083-44-9**
 129111-17-7
 RL: ANST (Analytical study)
 (detn. of famotidine and, in pharmaceuticals by spectrophotometry)
 IT 76824-35-6, Famotidine
 RL: ANST (Analytical study)
 (detn. of related compds. and, in pharmaceuticals by HPLC)
 IT **129083-44-9**
 RL: ANST (Analytical study)
 (detn. of famotidine and, in pharmaceuticals by spectrophotometry)
 RN 129083-44-9 HCAPLUS
 CN Guanidine, N,N'''-[dithiobis(methylene-4,2-thiazollediyl)]bis- (9CI) (CA INDEX NAME)



L58 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1985:166741 HCAPLUS
 DN 102:166741
 TI Sulfamylamide antisecretory agents
 IN Hoffman, Jacob M., Jr.
 PA Merck and Co., Inc. , USA
 SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

IC ICM C07D277-42

ICS C07D307-52

NCL 548193000

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 27

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4496737	A	19850129	US 1982-432219	19820927 <--
	ES 545561	A3	19860116	ES 1985-545561	19850726 <--
	ES 555773	A3	19870716	ES 1986-555773	19860606 <--
PRAI	US 1982-432219		19820927	<--	

OS CASREACT 102:166741

AB Title compds. R(CH₂)_nS(CH₂)₂C(:NR₁)NHR₂ [I; R = 5- or 6-membered (un)substituted heterocycle; R₁ = (un)substituted SO₂NH₂; R₂ = H, alkyl; n = 1-3] were prepd. by reacting CH₂:CHC(:NR₁)NHR₂, prepd. in 3 steps from R₃SCH₂CH₂C(:NR₂)OR₄ (R₂ as before; R₃, R₄ = alkyl, aryl, aralkyl), with R(CH₂)_nSH. Thus, MeSCH₂CH₂C(:NH)OMe was treated with H₂NSO₂NH₂ to give MeSCH₂CH₂C(NH₂):NSO₂NH₂ (II), which was oxidized with 3-CrC₆H₄C(O)OOH to the sulfoxide. The latter compd. was refluxed in EtOH in the presence of Et₃N to give CH₂:CHC(NH₂):NSO₂NH₂, which was treated with 5-(dimethylaminomethyl)furfurylthiol (III) to give I [R = 5-(dimethylaminomethylfuran-2-yl), R₁ = R₂ = H, n = 1] (IV). IV was also prepd. by treating II with III and Et₃N.

ST antisecretory sulfamylamidines; sulfamylamidines furanylmethylthio thiazolylmethylthio; furanylmethylthiosulfamylamidines; thiazolylmethylthiosulfamylamidines; guanidinothiazolylmethylthiosulfamylamidines

IT Synthons

(acrylsulfamylamidines, for heterocycylalkylthiosulfamylamidines antisecretory agents)

IT 80646-14-6 95853-51-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(addn. reaction of, with sulfamylacrylamidine)

IT 95853-46-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and addn. reactions of, with heterocycylalkylthiols)

IT 95853-50-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to free base)

IT 95853-47-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and elimination reaction of)

IT 95853-48-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 95853-49-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with sulfamide)

IT 76824-35-6P 81814-01-9P

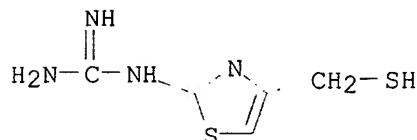
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 54974-63-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydrochloric acid and methanol)

IT 88046-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sulfamylacrylamidine)
 IT 95853-51-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addn. reaction of, with sulfamylacrylamidine)
 RN 95853-51-3 HCAPLUS
 CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L58 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1985:78888 HCAPLUS

DN 102:78888

TI Thiadiazole histamine H2-antagonists

IN Crenshaw, Ronnie R.; Algieri, Aldo A.

PA Bristol-Myers Co. , USA

SO U.S., 48 pp. Cont.-in-part of U.S. 4,394,508.

CODEN: USXXAM

DT Patent

LA English

IC C07D417-12

NCL 546209000

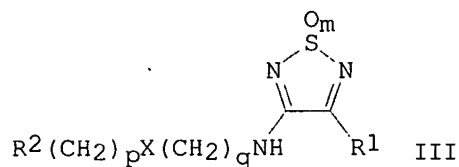
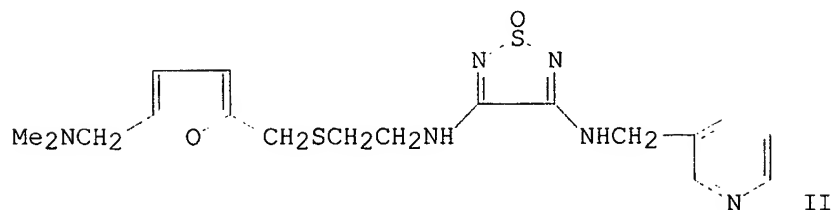
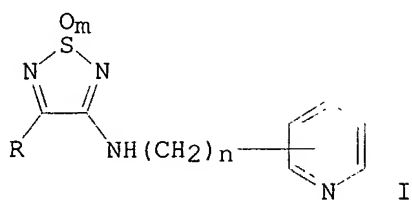
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4471122	A	19840911	US 1983-496321	19830519 <--
	ZA 8005250	A	19810930	ZA 1980-5250	19800825 <--
	FR 2476081	A1	19810821	FR 1980-18670	19800828 <--
	FR 2476081	B1	19850412		
	DK 8003718	A	19810305	DK 1980-3718	19800901 <--
	DK 160611	B	19910402		
	DK 160611	C	19910916		
	AU 8061942	A1	19810312	AU 1980-61942	19800901 <--
	AU 541849	B2	19850124		
	IL 60944	A1	19871130	IL 1980-60944	19800901 <--
	IL 75705	A1	19871130	IL 1980-75705	19800901 <--
	SE 8006148	A	19810415	SE 1980-6148	19800903 <--
	SE 449099	B	19870406		
	SE 449099	C	19870716		
	HU 29366	O	19840130	HU 1980-2170	19800903 <--
	HU 190669	B	19861028		
	SU 1396967	A3	19880515	SU 1980-2976950	19800903 <--
	HU 52490	A2	19900728	HU 1985-912	19800903 <--
	HU 201539	B	19901128		
	HU 57755	A2	19911230	HU 1989-3724	19800903 <--
	HU 205753	B	19920629		
	ES 494765	A1	19811001	ES 1980-494765	19800904 <--
	DD 153838	C	19820203	DD 1980-223725	19800904 <--
	CS 221977	P	19830429	CS 1980-6023	19800904 <--
	JP 63042624	B4	19880824	JP 1980-121855	19800904 <--
	US 4394508	A	19830719	US 1981-240034	19810303 <--
	FR 2486528	A1	19820115	FR 1981-15119	19810804 <--
	FR 2486528	B1	19841221		
	CS 246052	B2	19861016	CS 1981-6980	19810922 <--

GB 2132190	A1	19840704	GB 1983-18949	19830713 <--
GB 2132190	B2	19850103		
AT 8400645	A	19840715	AT 1984-645	19840227 <--
AT 377257	B	19850225		
AT 8400646	A	19850815	AT 1984-646	19840227 <--
AT 380019	B	19860325		
AT 8403301	A	19850715	AT 1984-3301	19841017 <--
AT 379806	B	19860310		
AT 8403302	A	19850715	AT 1984-3302	19841017 <--
AT 379807	B	19860310		
AU 8435396	A1	19850314	AU 1984-35396	19841113 <--
AU 563856	B2	19870723		
NO 160781	B	19890220	NO 1987-1421	19870406 <--
NO 160781	C	19890531		
NO 161737	B	19890612	NO 1987-1420	19870406 <--
NO 161737	C	19890920		
JP 63211272	A2	19880902	JP 1988-14800	19880127 <--
JP 05037990	B4	19930607		
JP 05078339	A2	19930330	JP 1991-235590	19910823 <--
JP 07010857	B4	19950208		
NL 9201236	A	19930301	NL 1992-1236	19920709 <--
NL 9201237	A	19930301	NL 1992-1237	19920709 <--
PRAI US 1979-72517		19790904 <--		
US 1980-117182		19800131 <--		
US 1980-163831		19800607 <--		
US 1981-240034		19810303 <--		
FR 1980-18670		19800828 <--		
IL 1980-60944		19800901 <--		
NL 1980-4967		19800901 <--		
GB 1980-28326		19800902 <--		
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AT 1980-4434		19800903 <--		
CS 1980-6023		19800904 <--		
AT 1984-646		19840227 <--		
OS CASREACT 102:78888				
GI				



- AB The thiadiazole derivs. I [R = halo, alkoxy, alkylthio, (un)substituted phenoxy, (un)substituted phenylthio] were prepd. Thus, 3-(aminomethyl)pyridine was treated with 3,4-dimethoxy-1,2,5-thiadiazole 1-oxide to give I (R = MeO, m = n = 1, 3-pyridyl), which was treated with 2-[(5-dimethylaminomethyl-2-furyl)methylthio]ethylamine to give the thiadiazole II. Thiadiazole derivs. III [R1 = HO, (un)substituted amino; R2 = heterocyclyl, Ph; X = CH2, S, O; m, p = 0, 2; q = 2-4] were also prepd. and their gastric antisecretory ED50 detd. in the pylorus-ligated rat test.
- ST histamine H2 antagonist aminothiadiazole oxide; ulcer treatment alkylaminothiadiazole dioxide; furylmethylthioethylaminothiadiazole ulcer treatment; thiadiazolediamine ulcer treatment; pyridylalkylaminothiadiazole oxide
- IT Antihistaminics
(alkylaminothiadiazole oxides)
- IT Ulcer
(inhibitors, alkylaminothiadiazole oxides)
- IT 541-41-3 1885-14-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminoacetonitrile deriv.)
- IT 25808-30-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
- IT 7170-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)
- IT 124-40-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of chloromethylfuran deriv.)
- IT 60-23-1 100-46-9, reactions 107-10-8, reactions 107-11-9 141-43-5, reactions 302-01-2, reactions 38585-75-0 66356-53-4 66356-54-5 66356-88-5 69340-31-4 69384-05-0 69384-24-3 71916-64-8 78442-21-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of dimethoxythiadiazole)
- IT 38585-67-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of dimethoxythiadiazoles)
- IT 67-62-9 74-89-5, reactions 75-04-7, reactions 109-85-3 110-89-4, reactions 110-91-8, reactions 123-75-1, reactions 124-22-1 765-30-0 2450-71-7 2516-47-4 2620-50-0 3731-51-9 3731-53-1 7803-49-8, reactions 69384-05-0 71916-66-0 73278-98-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of methoxythiadiazole deriv.)
- IT 87119-13-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of)
- IT 53227-32-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation by, of furfuryl alc.)
- IT 593-51-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation by, of methylfurfuryl alc.)
- IT 98-00-0 20416-16-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation of)
- IT 156-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminomethylfuranmethanol derivs.)
- IT 420-04-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminophenoxypropylphthalimide)

IT 37060-74-5 59608-97-8 78442-17-8 78442-48-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with cysteamine)

IT 50-00-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with furfuryl alc. and methylpropargylamine)

IT 15433-79-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with mercaptoethylthiadiazole deriv.)

IT 38603-72-4 38604-01-2 71916-64-8
RL: PROC (Process)
(conversion of, to free base)

IT 87766-25-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion to free base)

IT 534-07-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with (carbophenoxymethylamino)thioacetamide)

IT 36239-09-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with amidinothiourea)

IT 70-23-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aminothioacetamide deriv.)

IT 2114-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chloroformylacetate)

IT 598-52-7 6972-05-0 87766-22-1 87766-23-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with dichloroacetone)

IT 7719-09-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with oxalate diimide)

IT 30986-09-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with thionyl chloride)

IT 55904-37-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)

IT 59608-98-9P 78441-34-6P 78441-62-0P 78441-94-8P 78442-13-4P
78442-18-9P 78442-33-8P 78442-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination by, of dimethoxythiadiazole)

IT 87766-28-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination by, of methoxythiadiazole deriv.)

IT 55904-83-1P 78441-23-3P 78441-24-4P 78441-42-6P 78441-64-2P
78442-12-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination of)

IT 78442-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and chlorination of)

IT 87765-02-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and chloromethylation of)

IT 78441-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and condensation of, with aminoethanethiol)
 IT 78441-51-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with aminomethylfuranmethanol deriv.)
 IT 87107-74-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with cyanamide)
 IT 13242-91-6P 78441-33-5P **78441-93-7P** 78442-32-7P
 78442-43-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with cysteamine)
 IT 78441-36-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with cysteamine hydrochloride)
 IT 78442-24-7P 87765-03-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to free base)
 IT 87765-04-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and cyclocondensation of, with bromopyruvate)
 IT 78441-58-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and cyclocondensation of, with dichloroacetone)
 IT 78441-25-5P 78441-26-6P 78441-27-7P 78441-28-8P 78441-31-3P
 78441-32-4P 78441-35-7P 78441-44-8P 78441-46-0P 78441-47-1P
 78441-48-2P 78441-50-6P 78441-52-8P 78441-54-0P 78441-55-1P
 78441-56-2P 78441-65-3P 78441-70-0P 78441-71-1P 78441-72-2P
 78441-73-3P 78441-79-9P 78441-80-2P 78441-81-3P 78441-82-4P
 78441-83-5P 78441-84-6P 78441-85-7P 78441-86-8P 78441-87-9P
 78441-88-0P 78441-89-1P 78441-90-4P 78441-95-9P 78441-96-0P
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 78467-82-0P 78467-83-1P 78467-85-3P 81074-53-5P 87107-89-9P
 87107-90-2P 87107-91-3P 87107-92-4P 87107-93-5P 87107-94-6P
 87107-95-7P 87107-96-8P 87107-98-0P 87119-17-3P 87119-18-4P
 87765-05-7P 87766-21-0P 87766-24-3P 87766-26-5P 87785-45-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and gastric acid secretion inhibition by)
 IT 87766-27-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and hydrazinolysis of)
 IT 94567-20-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with [(dimethylaminomethylseryl)methylthio]eth
 ylamine)
 IT 78441-61-9P 78441-68-6P 78441-92-6P 78442-10-1P 78442-42-9P
 87107-73-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and redn. of)
 IT 78441-39-1P 78441-59-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and substitution reaction of, with cysteamine)
 IT 78441-57-3P 78441-66-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and sulfuration of)

IT 66356-58-9P 72158-79-3P 78441-37-9P 78441-40-4P 78441-45-9P
 78441-52-8P 78441-53-9P 78441-63-1P 78441-69-7P 78441-70-0P
 78441-75-5P 78441-76-6P 78441-78-8P 78441-80-2P 78441-82-4P
 78441-83-5P 78441-84-6P 78442-30-5P 78442-37-2P 78442-44-1P
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 87119-15-1P 87766-24-3P 87766-29-8P 87766-30-1P 87766-31-2P
 94567-21-2P 94567-22-3P 94567-23-4P 94567-24-5P 94567-25-6P
 94567-26-7P 94567-27-8P 94567-28-9P 94567-29-0P 94567-30-3P
 94567-31-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 71916-64-8 71916-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with dimethoxythiadiazole dioxide)

IT 3731-52-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with dimethoxythiadiazole oxide)

IT 66356-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methoxy(pyridylmethylamino)thiadiazole oxide)

IT 58677-34-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (redn. of)

IT 554-84-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with bromopropylphthalimide)

IT 3914-42-9 62642-47-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with cysteamine)

IT 5460-29-7

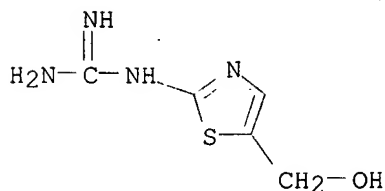
RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with nitrophenol)

IT 78441-93-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with cysteamine)

RN 78441-93-7 HCAPLUS

CN Guanidine, [5-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L58 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1983:594974 HCAPLUS

DN 99:194974

TI Histamine H2-antagonists useful in treating peptic ulcers

IN Crenshaw, Ronnie R.; Algieri, Aldo A.

PA Bristol-Myers Co. , USA

SO U.S., 52 pp. Cont.-in-part of U.S. Ser. No. 163,831, abandoned.

CODEN: USXXAM

DT Patent

LA English

IC C07D417-12; C07D285-10

NCL 546209000

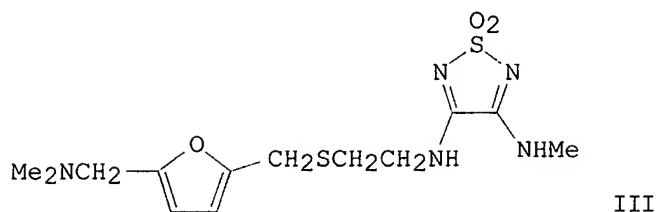
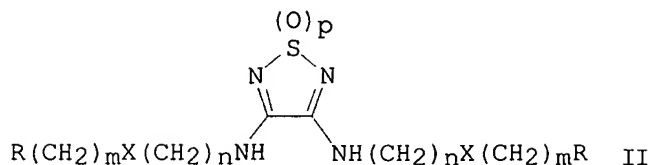
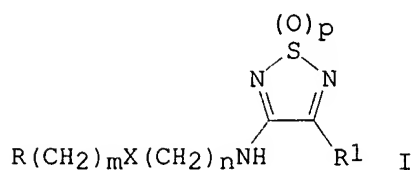
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	FR 2476081	B1	19850412		
	FI 8002740	A	19810305	FI 1980-2740	19800901 <--
	FI 76795	B	19880831		
	FI 76795	C	19881212		
	DK 8003718	A	19810305	DK 1980-3718	19800901 <--
	DK 160611	B	19910402		
	DK 160611	C	19910916		
	NL 8004967	A	19810306	NL 1980-4967	19800901 <--
	NL 189197	B	19920901		
	NL 189197	C	19930201		
	AU 8061942	A1	19810312	AU 1980-61942	19800901 <--
	AU 541849	B2	19850124		
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	NO 160003	B	19881121		
	NO 160003	C	19890301		
	GB 2067987	A	19810805	GB 1980-28326	19800902 <--
	GB 2067987	B2	19840711		
	SE 8006148	A	19810415	SE 1980-6148	19800903 <--
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	SE 449099	C	19870716		
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	SU 1396967	A3	19880515	SU 1980-2976950	19800903 <--
	HU 52490	A2	19900728	HU 1985-912	19800903 <--
	HU 201539	B	19901128		
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	HU 205753	B	19920629		
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	CS 221977	P	19830429	CS 1980-6023	19800904 <--
	CS 235951	B2	19850515	CS 1981-6979	19800904 <--
	JP 63042624	B4	19880824	JP 1980-121855	19800904 <--
	US 4374248	A	19830215	US 1981-276586	19810623 <--
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	FR 2486528	B1	19841221		
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SE 456580	C	19890209		
SE 8403108	A	19840608	SE 1984-3108	19840608 <--
SE 456582	B	19881017		
SE 456582	C	19890209		
SE 8403109	A	19840608	SE 1984-3109	19840608 <--
SE 456581	B	19881017		
SE 456581	C	19890209		
SE 8403111	A	19840608	SE 1984-3111	19840608 <--
SE 461733	B	19900319		
SE 461733	C	19900712		
AT 8403301	A	19850715	AT 1984-3301	19841017 <--
AT 379806	B	19860310		
AT 8403302	A	19850715	AT 1984-3302	19841017 <--
AT 379807	B	19860310		
AU 8435396	A1	19850314	AU 1984-35396	19841113 <--
AU 563856	B2	19870723		
NO 8602501	A	19810305	NO 1986-2501	19860623 <--
NO 162664	B	19891023		
NO 162664	C	19900131		
NO 160781	B	19890220	NO 1987-1421	19870406 <--
NO 160781	C	19890531		
NO 161737	B	19890612	NO 1987-1420	19870406 <--
NO 161737	C	19890920		
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JP 05037990	B4	19930607		
DK 9002689	A	19901109	DK 1990-2689	19901109 <--
DK 164363	B	19920615		
DK 164363	C	19921102		
DK 9002690	A	19901109	DK 1990-2690	19901109 <--
DK 164700	B	19920803		
DK 164700	C	19921221		
DK 9002691	A	19901109	DK 1990-2691	19901109 <--
DK 164702	B	19920803		
DK 164702	C	19921221		
JP 05078339	A2	19930330	JP 1991-235590	19910823 <--
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NL 9201236	A	19930301	NL 1992-1236	19920709 <--
NL 9201237	A	19930301	NL 1992-1237	19920709 <--
PRAI US 1979-72517		19790904	<--	
US 1980-117182		19800131	<--	
US 1980-163831		19800607	<--	
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IL 1980-60944		19800901	<--	
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GB 1980-28326		19800902	<--	
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CS 1980-6023		19800904	<--	
US 1981-240034		19810303	<--	
AT 1984-646		19840227	<--	
OS CASREACT 99:194974				
GI				



- AB Thiadiazoles I and II [R = Ph, heterocyclyl, i.e., furyl, thienyl, thiazolyl substituted by alkyl, HO, halo, NH₂, alkoxy, guanidinoalkyl, aminoalkyl, heterocyclylalkyl; R₁ = HO, R₂R₃N (R₂,R₃ = H, alkyl, alkenyl, hydroxyalkyl, heterocyclylalkyl, substituted pyridylalkyl, Ph, substituted Ph; m = 0-2; n = 2-4; p = 1, 2; X = CH₂, S, O, substituted HN] were prepd. by amination of dimethoxythiadiazoles and possessed histamine H₂ antagonist and gastric acid secretion inhibiting activities. Thus, treatment of 3,4-dimethoxy-1,2,5-thiadiazole 1,1-dioxide with 2-[(5-dimethylaminomethyl-2-furyl)methylthio]ethylamine in MeOH at 8-10.degree. for 15 min and then with MeNH₂ for 10 min gave the diaminothiadiazolediamine III. In the 2 h pylorus ligated rat test III possessed an ED₅₀ of 0.69 .mu.moles/kg compared to 9 .mu.moles/kg for cimetidine.
- ST histamine H₂ antagonist aminothiadiazolediamine; ulcer treatment alkylaminothiadiazolediamine; furylmethylthioethylaminothiadiazolediamine ulcer treatment; thiadiazolediamine ulcer treatment
- IT Antihistaminics
(alkylaminothiadiazolediamine oxides)
- IT Ulcer
(inhibitors, alkylaminothiadiazolediamine oxides)
- IT 541-41-3 1885-14-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminoacetonitrile deriv.)
- IT 25808-30-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
- IT 7170-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)
- IT 124-40-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of chloromethylfuran deriv.)
- IT 60-23-1 100-46-9, reactions 107-10-8, reactions 107-11-9 141-43-5, reactions 302-01-2, reactions 38585-75-0 66356-53-4 66356-54-5 66356-88-5 69340-31-4 69384-05-0 69384-24-3 71916-64-8 78442-21-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of dimethoxythiadiazole)

IT 38585-67-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of dimethoxythiadiazoles)

IT 67-62-9 74-89-5, reactions 75-04-7, reactions 109-85-3 110-89-4,
reactions 110-91-8, reactions 123-75-1, reactions 124-22-1
765-30-0 2450-71-7 2516-47-4 2620-50-0 3731-51-9 3731-53-1
7803-49-8, reactions 69384-05-0 71916-66-0 73278-98-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of methoxythiadiazole deriv.)

IT 87119-13-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of)

IT 53227-32-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation by, of furfuryl alc.)

IT 593-51-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation by, of methylfurfuryl alc.)

IT 98-00-0 20416-16-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminomethylation of)

IT 156-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminomethylfuranmethanol derivs.)

IT 420-04-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminophenoxypropylphthalimide)

IT 37060-74-5 59608-97-8 78442-17-8 78442-48-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with cysteamine)

IT 50-00-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with furfuryl alc. and methylpropargylamine)

IT 15433-79-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with mercaptoethylthiadiazole deriv.)

IT 38603-72-4 38604-01-2 71916-64-8
RL: PROC (Process)
(conversion of, to free base)

IT 87766-25-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion to free base)

IT 534-07-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with (carbophenoxymethylamino)thioacetamide)

IT 36239-09-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with amidinothiourea)

IT 70-23-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aminothio acid amide deriv.)

IT 2114-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chloroformylacetate)

IT 598-52-7 6972-05-0 87766-22-1 87766-23-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with dichloroacetone)

IT 7719-09-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with oxalate diimide)

IT 30986-09-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with thionyl chloride)

IT 55904-37-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)

IT 59608-98-9P 78441-34-6P 78441-62-0P 78441-94-8P 78442-13-4P
78442-18-9P 78442-33-8P 78442-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination by, of dimethoxythiadiazole)

IT 87766-28-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination by, of methoxythiadiazole deriv.)

IT 55904-83-1P 78441-23-3P 78441-24-4P 78441-42-6P 78441-64-2P
78442-12-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and amination of)

IT 78442-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and chlorination of)

IT 87765-02-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and chloromethylation of)

IT 78441-51-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with aminomethylfuran methanol deriv.)

IT 78441-33-5P 78442-43-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with cysteamine)

IT 78441-36-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with cysteamine hydrochloride)

IT 78441-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with aminoethanethiol)

IT 87107-74-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with cyanamide)

IT 13242-91-6P **78441-93-7P** 78442-32-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with cysteamine)

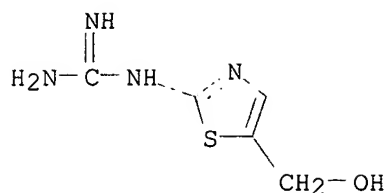
IT 78442-24-7P 87765-03-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to free base)

IT 87765-04-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation with bromopyruvate)

IT 78441-58-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation with dichloroacetone)

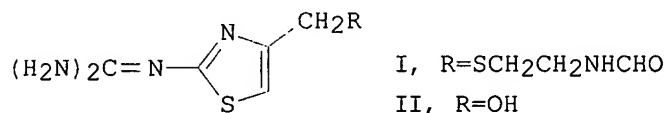
IT 78441-27-7P 78441-28-8P 78441-31-3P 78441-35-7P 78441-44-8P
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78442-00-9P 78442-01-0P 78442-02-1P 78442-03-2P 78442-04-3P
78442-05-4P 78442-06-5P 78442-07-6P 78442-08-7P 78442-14-5P
78442-20-3P 78442-22-5P 78442-23-6P 78442-25-8P 78442-26-9P
78442-27-0P 78442-28-1P 78442-31-6P 78442-34-9P 78442-35-0P

78442-36-1P 78442-38-3P 78442-39-4P 78442-40-7P 78442-41-8P
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 81074-53-5P 87107-89-9P 87107-90-2P 87107-91-3P 87107-92-4P
 87107-93-5P 87107-94-6P 87107-95-7P 87107-96-8P 87107-98-0P
 87119-17-3P 87119-18-4P 87765-05-7P 87766-21-0P 87766-24-3P
 87766-26-5P 87785-45-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and gastric acid secretion inhibition by)
 IT 78441-25-5P 78441-26-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and gastric acids secretion inhibition by)
 IT 78441-32-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and gastric secretion inhibition by)
 IT 87766-27-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and hydrazinolysis of)
 IT 78441-61-9P 78441-68-6P 78441-92-6P 78442-10-1P 78442-42-9P
 87107-73-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and redn. of)
 IT 78441-39-1P 78441-59-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution reaction with cysteamine)
 IT 78441-57-3P 78441-66-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and sulfuration of)
 IT 66356-58-9P 72158-79-3P 78441-37-9P 78441-40-4P 78441-45-9P
 78441-52-8P 78441-53-9P 78441-63-1P 78441-69-7P 78441-70-0P
 78441-75-5P 78441-76-6P 78441-78-8P 78441-80-2P 78441-82-4P
 78441-83-5P 78441-84-6P 78442-30-5P 78442-37-2P 78442-44-1P
 78467-80-8P 78467-84-2P 87107-68-4P 87107-69-5P 87107-89-9P
 87107-95-7P 87107-97-9P 87119-15-1P 87766-24-3P 87766-29-8P
 87766-30-1P 87766-31-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 58677-34-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (redn. of)
 IT 554-84-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with bromopropylphthalimide)
 IT 3914-42-9 62642-47-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with cysteamine)
 IT 5460-29-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with nitrophenol)
 IT 78441-93-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation with cysteamine)
 RN 78441-93-7 HCAPLUS
 CN Guanidine, [5-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L58 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1983:488191 HCAPLUS
 DN 99:88191
 TI 2-Guanidino-4-[[(2-formamidoethyl)thio]methyl]thiazole
 PA Shionogi and Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC C07D277-48
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 58072571	A2	19830430	JP 1981-172391	19811027 <--
	JP 01039428	B4	19890821		
	US 4492794	A	19850108	US 1983-488821	19830426 <--
PRAI	JP 1981-172391		19811027 <--		
OS	CASREACT 99:88191				
GI					



AB The title compd. (I) was prepd. by reaction of II with (SCH₂CH₂NHCHO)₂ (III) in the presence of a phosphorus compd. Thus, stirring 0.157 g II, 1.87 g III, 1.82 g Bu₃P, and 1.5 mL pyridine at room temp. for 8 h and allowing the resulting mixt. to stand overnight gave, after treatment with maleic acid, 0.81 g I maleate, which had antihistaminic activity (no data).

ST guanidinoformamidoethylthiomethylthiazole antihistaminic prepn; thiazole guanidino formamidoethylthiomethyl

IT Antihistaminics
 (guanidino[[(formamidoethyl)thio]methyl]thiazole)

IT Condensation reaction
 (of thiazolemethanol derivs. with bis(formamidoethyl) disulfide)

IT 86794-43-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with thiazolemethanol deriv.)

IT 2114-02-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with chlorooxopropylacetate in prepn. of thiazole derivs.)

IT 70-23-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with guanylthiourea)

IT 106-89-8, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of acetic acid)

IT **86794-42-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with bis(formamidoethyl) disulfide)

IT 40235-68-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization with formylthiourea)

IT 86794-41-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and hydrolysis of)

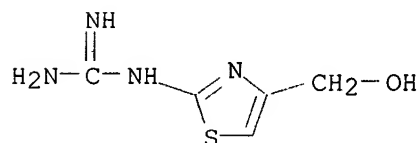
IT 24573-30-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and oxidn. of)

IT 81152-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **86794-42-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with bis(formamidoethyl) disulfide)

RN 86794-42-5 HCAPLUS

CN Guanidine, [4-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L58 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1976:44102 HCAPLUS

DN 84:44102

TI Cephem derivatives

PA Hoechst A.-G., Fed. Rep. Ger.

SO Neth. Appl., 104 pp.

CODEN: NAXXAN

DT **Patent**

LA Dutch

IC C07D; A61K

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	NL 7415285	A	19750602	NL 1974-15285	19741122	<--
	DE 2359544	A1	19751030	DE 1973-2359544	19731129	<--
	CA 1040621	A1	19781017	CA 1974-212430	19741028	<--
	ES 432221	A1	19761101	ES 1974-432221	19741123	<--
	FI 7403433	A	19750530	FI 1974-3433	19741127	<--
	DD 117076	C	19751220	DD 1974-182617	19741127	<--
	AU 7475812	A1	19760527	AU 1974-75812	19741127	<--
	US 4016159	A	19770405	US 1974-527704	19741127	<--
	NO 7404296	A	19750530	NO 1974-4296	19741128	<--
	JP 50088088	A2	19750715	JP 1974-135961	19741128	<--
	DK 7406195	A	19750728	DK 1974-6195	19741128	<--
	ZA 7407594	A	19751231	ZA 1974-7594	19741128	<--
	GB 1469448	A	19770406	GB 1974-51644	19741128	<--
	AT 7409534	A	19770515	AT 1974-9534	19741128	<--
	AT 341087	B	19780125			

CH 611305 A 19790531 CH 1974-15814 19741128 <--
 CH 611307 A 19790531 CH 1978-2464 19741128 <--
 BE 822780 A1 19750529 BE 1974-151010 19741129 <--
 SE 7414994 A 19750530 SE 1974-14994 19741129 <--
 FR 2252850 A1 19750627 FR 1974-39302 19741129 <--
 HU 169852 P 19770228 HU 1974-HO1747 19741129 <--
 AT 349635 B 19790410 AT 1977-2700 19770418 <--
 PRAI DE 1973-2359544 19731129 <--
 AT 1974-9534 19770418 <--
 GI For diagram(s), see printed CA Issue.
 AB Cephalosporins I (R-R2 = H, alkyl; RR1 = alkylene; X = p-C6H4, substituted p-phenylene, p-NHC6H4, p-C6H4O, p-NHC6H4O, 2,5-thienylidene, 2,5-thienylideneoxy; R3 = heterocyclic) were prepd. Thus 4-H2NC(:NH)C6H4CH2CO2H was converted to its chloride and treated with 7-amino-3-(1,3,4-thiadiazol-2-ylthiomethyl)-3-cephem-4-carboxylic acid to give I (R-R2 = H, R3 = 1,3,4-thiadiazol-2-yl, X = p-C6H4).
 ST amidinophenylacetamidocephem; cephem amidinophenylacetamido
 IT 957-68-6 24209-43-6 30246-33-4 37506-38-0 37506-39-1 51126-83-1
 51646-50-5 58016-62-9 58016-82-3 58016-84-5 58016-87-8
 58017-41-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of)
 IT 51322-35-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of aminocephems by)
 IT 3956-33-0 39244-83-2 51322-33-9 51322-34-0 51322-35-1
 51322-37-3 58016-68-5 58016-88-9 58017-80-4 58017-85-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of)
 IT 58017-86-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acylation of aminocephalosporanates by)
 IT 58017-81-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acylation of aminocephalosporanic acid by)
 IT 7035-88-3P 32098-03-6P 32245-16-2P 51322-25-9P 58016-58-3P
 58016-89-0P 58103-79-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acylation of aminocephems by)
 IT 32098-02-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reaction of, with aminocephems)
 IT 58017-82-6P 58017-87-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reaction of, with heterocyclic thiols)
 IT 58016-57-2P 58016-59-4P 58016-60-7P 58016-61-8P 58016-63-0P
 58016-64-1P 58016-65-2P 58016-66-3P 58016-67-4P 58016-69-6P
 58016-70-9P 58016-71-0P 58016-72-1P 58016-73-2P 58016-74-3P
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 58016-80-1P 58016-81-2P 58016-83-4P 58016-85-6P 58016-86-7P
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 58017-91-7P 58103-78-9P 58103-80-3P 58103-81-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 20069-34-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acetoxycephems)

IT 1121-31-9 2127-09-5 2180-05-4 2382-96-9 3581-91-7 33120-79-5
 36988-21-3

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acylaminocephalosporanate)

IT 60-56-0 86-93-1 96-53-7 141-90-2 149-30-4 2349-67-9 2637-34-5
 2637-37-8 3004-42-0 4343-75-3 4556-23-4 7271-45-6 20939-15-5
 20939-16-6 22325-27-5 24521-48-0 31130-16-2 35071-17-1
 58017-09-7 58017-11-1 58017-26-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acylaminocephalosporanates)

IT 615-76-9 2103-88-0 5685-05-2 5685-06-3 7271-44-5 18686-82-3
 29490-19-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acylaminocephalosporanic acids)

IT 39244-85-4 58023-74-8 58023-75-9

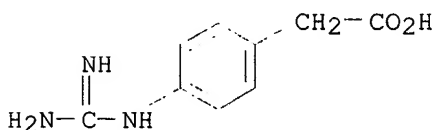
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with heterocyclic thiols)

IT 3956-33-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of)

RN 3956-33-0 HCAPLUS

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1974:565375 HCAPLUS

DN 81:165375

TI Synthetic inhibitors of serine proteinases. 3. Inhibitory effect of
 basically substituted phenylcarboxylic acid ester against trypsin,
 plasmin, and thrombin

AU **Stuerzebecher, J.**; Markwardt, F.; Richter, P.; Wagner, G.;
 Walsmann, P.; Landmann, H.

CS Inst. Pharmakol. Toxikol., Med. Akad. Erfurt, Erfurt, Ger. Dem. Rep.

SO Pharmazie (1974), 29(5), 337-8

CODEN: PHARAT; ISSN: 0031-7144

DT Journal

LA German

CC 7-3 (Enzymes)

AB The inhibitory strength of 12 Ph esters of substituted benzoic acids and

of 11 guanidinophenyl acetic acids (I) and guanidinocinnamic acids (II) and their ester was detd. on the hydrolysis of N.alpha.-benzoyl-DL-arginine-4-nitroanilide by the title enzymes and on the hydrolysis of N.alpha.-benzoyl-L-arginine Et ester by trypsin [9002-07-7] and on the coagulation of fibrinogen by thrombin [9002-04-4]. All inhibitors were used as salts. 4-Guanidinobenzoic acid Ph ester [35695-21-7] had the strongest anti-trypsin, anti-plasmin [9001-90-5], and anti-thrombin activity. I and II and their esters were less inhibitory than the corresponding amidino derivs.

ST serine protease inhibition; trypsin inhibition phenylcarboxylate ester; plasmin inhibition phenylcarboxylate ester; thrombin inhibition phenylcarboxylate ester; phenylcarboxylate ester enzyme inhibition

IT 9001-90-5 9002-04-4 9002-07-7

RL: PROC (Process)

(inhibition of, by phenylcarboxylic acid esters)

IT 52820-37-8

RL: BIOL (Biological study)

(serine proteinase inhibition by)

IT 3956-33-0 15676-15-0 35695-21-7 39244-83-2

50466-07-4 50466-20-1 50466-32-5 52779-42-7 52779-44-9

52779-46-1 52779-48-3 52779-50-7 52779-52-9 52798-10-4

52798-68-2 52798-92-2 52820-31-2 52820-33-4 52820-34-5

52820-35-6 52820-36-7 52820-38-9 52820-39-0 52820-40-3

52820-41-4 52820-42-5 52820-43-6 52820-44-7 52820-45-8

52820-46-9 52820-47-0 52820-48-1 53002-19-0

RL: BIOL (Biological study)

(serine proteinases inhibition by)

IT 3956-33-0 15676-15-0 52820-39-0

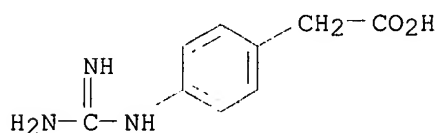
52820-41-4

RL: BIOL (Biological study)

(serine proteinases inhibition by)

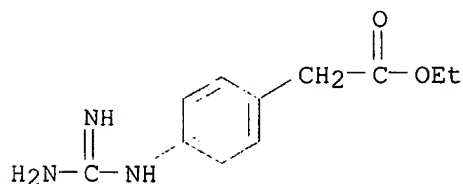
RN 3956-33-0 HCAPLUS

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



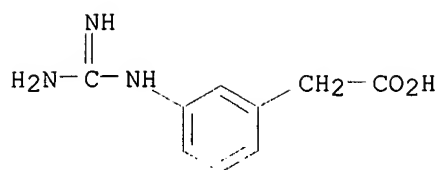
RN 15676-15-0 HCAPLUS

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

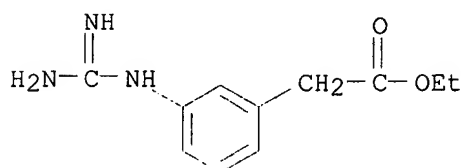


RN 52820-39-0 HCAPLUS

CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



RN 52820-41-4 HCAPLUS
 CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



L58 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1973:147591 HCAPLUS

DN 78:147591

TI Thiol esters of guanidine-substituted carboxylic acids

IN Iro, Hiroyuki; Sasaki, Yutaro; Miyamoto, Shigetoshi; Kayama, Naohiro; Kajiwara, Ikuo; Iguchi, Yoichi; Sakaguchi, Kimiko; Hama, Kazuaki; Yo, Ikuko; et al.

PA Ono Pharmaceutical Co., Ltd.

SO Ger. Offen., 27 pp.

CODEN: GWXXBX

DT Patent

LA German

IC C07C; A61K

CC 25-18 (Noncondensed Aromatic Compounds)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	DE 2240664	A1	19730308	DE 1972-2240664	19720818 <--
	JP 48029732	A2	19730419	JP 1971-63277	19710819 <--
	JP 55042076	B4	19801028		
	JP 49024917	A2	19740305	JP 1972-64761	19720628 <--
	JP 56003345	B4	19810124		
	US 3824267	A	19740716	US 1972-280485	19720814 <--
	HU 164485	P	19740228	HU 1972-00185	19720817 <--
	BE 787759	A1	19721218	BE 1972-121134	19720818 <--
	FR 2150802	A1	19730413	FR 1972-29666	19720818 <--
	SU 468405	D	19750425	SU 1972-1822859	19720818 <--
PRAI	SE 380794	B	19751117	SE 1972-10795	19720818 <--
	GB 1362918	A	19740807	GB 1972-38956	19720821 <--
	JP 1971-63277		19710819 <--		
	JP 1972-64761		19720628 <--		

AB The title guanidino esters $\text{H}_2\text{NC}(:\text{NH})\text{NHQC}(\text{O})\text{SR}$ (I: Q = p-C₆H₄, p-CH₂C₆H₄CH₂, 1,4-cyclohexylene, CH₂-1,4-cyclohexylene, (CH₂)_n; n = 4, 5, 6; R = alkyl, cyclohexyl, 8-carbethoxy-1-naphthyl, Ph, or phenyl substituted by ester, amide, nitro, etc.), useful as antiviral agents against influenza, were obtained in to form of phosphate, coarbonate, p-tosylate, or sulfate salts by treating a guanidino acid with SOCl₂, a mercaptan, and a salt of the desired acid. Thus, $\text{H}_2\text{NC}(:\text{NH})\text{NH}(\text{CH}_2)_5\text{CO}_2\text{H}$ (II) was treated with SOCl₂ p-HSC₆H₄CO₂Et and H₃PO₄ to give $\text{H}_2\text{NC}(:\text{NH})\text{NH}(\text{CH}_2)_5\text{C}(\text{O})\text{SC}_6\text{H}_4\text{CO}_2\text{Et}$ -p.H₃PO₄, and II with SOCl₂, Me(CH₂)₄SH, and NaHCO₃ gave

H2NC(:NH)NH(CH2)5C(O)S(CH2)4Me.H2 CO3, which was then converted to the phosphate salt.

ST guanidino ester antiviral influenza; thiol guanidinocarboxylate; benzoate guanidinoacylthio

IT Virucides and Virustats
(against influenza, guanidino-contg. thiocarboxylate esters as)

IT Thiols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, by guanidino-substituted carboxylic acids)

IT Influenza
(guanidino-contg. thiocarboxylate esters in treatment of)

IT Esters, preparation
RL: PREP (Preparation)
(guanidino-contg. thiocarboxylates)

IT 41651-94-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of thiols)

IT 108-98-5 110-66-7 28276-32-6 41651-93-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, by guanidino-substituted carboxylic acids)

IT 41651-37-0P 41651-38-1P 41651-39-2P 41651-40-5P 41651-41-6P
41651-42-7P 41651-43-8P 41651-44-9P 41651-45-0P 41651-46-1P
41651-47-2P 41651-48-3P 41651-49-4P 41651-50-7P 41651-51-8P
41651-52-9P 41651-53-0P 41651-54-1P 41651-55-2P 41651-56-3P
41651-57-4P 41651-58-5P 41651-59-6P 41651-60-9P 41651-61-0P
41651-62-1P 41651-63-2P 41651-65-4P 41651-66-5P 41651-67-6P
41651-68-7P 41651-69-8P 41651-70-1P 41651-71-2P 41651-72-3P
41651-73-4P 41651-74-5P 41651-75-6P 41651-76-7P 41651-77-8P
41651-78-9P 41651-79-0P 41651-80-3P 41651-81-4P 41651-82-5P
41651-83-6P 41651-84-7P 41729-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

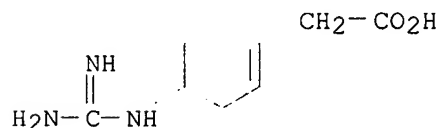
IT 7719-09-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with guanidino-substituted carboxylic acids)

IT 3956-33-0 6659-35-4 16060-65-4 41651-86-9 41651-87-0
41651-88-1 41651-90-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionylchloride and thiols)

IT 3956-33-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionylchloride and thiols)

RN 3956-33-0 HCAPLUS

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1970:43668 HCAPLUS

DN 72:43668

TI Antibacterial guanidinoarylpenicillins

IN Patchett, Arthur A.; Rogers, Edward F.; Leanza, William J.

PA Merck and Co., Inc.

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English
 IC C07D; C07C
 NCL 260518000
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3479401	A	19691118	US 1966-561052	19660628 <--
PRAI	US 1966-561052		19660628	<--	

GI For diagram(s), see printed CA Issue.

AB The title compds. (I), useful in inhibiting gram-pos. bacteria, are prepd. by treating 6-aminopenicillanic acid or its derivs. with a guanidinoaryl or guanidinomethylaryl-substituted carboxylic acid. Thus, 1.5 g p-NH₂C₆H₄CO₂H and 1.62 g BzNHCN in 5 ml EtOH was evapd., and the residue stirred in 5% aq. NaHCO₃ soln. and filtered, 4 equivs. NaOH added followed by refluxing and the soln. acidified with AcOH to give p-NH₂C(:NH)NHC₆H₄COC₁.HCl. This (650 mg) was added to 648 mg 6-aminopenicillanic acid in 8.5% aq. NaHCO₃ (pH 7.8) to ppt. I (R = p-NH₂C(:NH)NHC₆H₄CO). I [R = 5-methyl-3-(4-guanidinophenyl)-4-isoxazolyl] was similarly prepd. A mixt. of 1.4 g p-NH₂C₆H₄OCH₂-CO₂H, 2 ml Me₂NCHO, 1.4 g MeSC(:NH)NHNO₂, and aq. NaOH contg. 10 equiv. was stirred at 60.degree. for 1.5 hr to give p-O₂NNHC(:NH)NHC₆H₄OCH₂CO₂H, m. 239.degree. (decompn.). This (7.3 g) in 450 ml 90% aq. MeOH was hydrogenated at 40 psig over 4.5 g 10% Pd/C to produce [p-NH₂C(:NH)NHC₆H₄OCH₂CO₂H].HCl, m. 170.degree.. This (0.5 g) in 0.87 ml Me₂NCHO was added to 518 mg dicyclohexylcarbodiimide and 779 mg benzyl 6-aminopenicillanate in 0.87 ml Me₂NCHO to give I (R = p-NH₂C(:NH)NHC₆H₄OCH₂CO) benzyl ester hydrochloride. This was hydrogenated in MeOH at 40 psig to give the corresponding I. I (R = p-NH₂C(:NH)NHCH₂C₆H₄CO and R = p-NH₂C(:NH)NHCH₂C₆H₄CH₂CO) was similarly prepd. To 6.04 g p-NH₂C₆H₄CH₂CO₂H in 50 ml H₂O and 15 ml 2.7N NaOH was added 5.4 g powd. MeSC(:NH)NHNO₂ to give 4.4 g p-O₂NNHC(:NH)NHC₆H₄CH₂CO₂H, m. 188-90.degree.. This (2.0 g) in 75 ml MeOH was refluxed with 1 g Raney Ni and hydrogenated at 40 psig and 25.degree. to yield p-NH₂C(:NH)NHC₆H₄CH₂CO₂H, m. 320-2.degree. (decompn.). This (0.2 g) was treated with 0.3 ml SOCl₂ at room temp. to give [p-NH₂C(:NH)NHC₆H₄CH₂COC₁].HCl, m. 127-30.degree. (decompn.). The latter was added to 0.23 g Na 6-aminopenicillanate in 2 ml 1:1 tetrahydrofuran-H₂O, 2 ml 0.5N aq. NaHCO₃ added, and the mixt. stirred at 25.degree. for 10 min to yield I (R = p-NH₂C(:NH)NHC₆H₄CH₂CO), m. 195-200.degree.. 3-Bromo-2,6-dimethoxybenzoic acid (11 g), 3.7 g K₂CO₃, and 6 ml PhC₂H₅Br in 100 ml Me₂CO was refluxed 20 hr to give the benzyl ester. This (11 g) was treated with NaNH₂ (from 1.2 g Na and 200 ml liq. NH₃) to give benzyl 4-amino-2,6-dimethoxybenzoate, m. 115-16.degree., which (547 mg) was heated in 5 ml EtOH with 324 mg BzNHCN for 30 min to yield 2,6-dimethoxy-4-guanidinobenzoic acid hydrochloride, m. 220.degree. (decompn.). This was used for prepn. of I (R = 2,6-dimethoxy-4-guanidinobenzoyl).

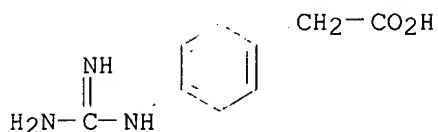
ST antibacterial penicillins; penicillins antibacterial; guanidino aryl penicillins; benzoyl penicillins

IT Benzohydroximoyl chloride, p-nitro-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 56-91-7P 1129-37-9P 3956-33-0P 4085-41-0P 4255-81-6P
 7035-77-0P 7035-78-1P 7035-79-2P 7035-80-5P 7035-81-6P
 7035-82-7P 7035-83-8P 7035-84-9P 7035-86-1P 7035-88-3P
 7035-90-7P 7035-91-8P 7035-92-9P 7123-64-0P 14373-63-8P
 16060-65-4P 25614-22-6P 25614-24-8P 25647-23-8P 25647-25-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 3956-33-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 3956-33-0 HCAPLUS
 CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1966:447730 HCAPLUS

DN 65:47730

OREF 65:8919g-h,8920a-h,8921a-b

TI 5-Methyl-3-(p-guanidinophenyl)-4-isoxazolylicarboxylic acid

IN Patchett, Arthur A.; Rogers, Edward F.; Leanza, William J.

PA Merck & Co., Inc.

SO 6 pp.

DT Patent

LA Unavailable

NCL 260307000

CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

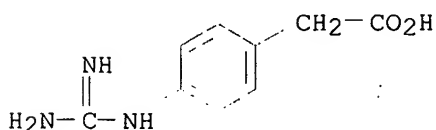
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3257411		19660621	US	19630614 <--
AB	<p>The title compd. (I) and similar carboxylic acids are prepd. and condensed with 6-aminopenicillanic acid (II) to give penicillin which are esp. effective against gram neg. bacilli. p-Guanidinobenzoyl chloride-HCl (III) (.apprx.650 mg.) is added in small portions to a stirred soln. of 648 mg. II in 8.5% aq. NaHCO₃ soln. keeping the pH in the range of 7-8 by intermediate addn. of a satd. NaHCO₃ soln. The mixt. is stirred .apprx.45 min. and the pptd. p-guanidinophenylpenicillin (IV) recrystd. from Me₂CO-H₂O; IV inhibits Staphylococcus aureus (S.a.) at a concn. of 3.9 mg./ml. III is prepd. by evapg. a soln. of 1.5 g. p-H₂NC₆H₄CO₂H and 1.62 g. BzNHCN in 5 ml. EtOH on a steam bath and distg. off another 5 ml. EtOH. The residue is stirred 1 hr. in 5% aq. NaHCO₃, 4 equiv. NaOH added to the filtered soln., the mixt. refluxed 20 min., decolorized with C, another 6 equiv. NaOH added and the mixt. kept 0.5 hr. at 25.degree. and acidified with AcOH, pptg. p-guanidinobenzoic acid which is treated with 5 ml. SOCl₂ and 3 drops C₅H₅N to give 537 mg. III. I (400 mg.) and 4 ml. SOCl₂ refluxed .apprx.15 min., the excess SOCl₂ evapd. in vacuo, the residual acid chloride dissolved in 5 ml. dry Me₂CO and added to 283 mg. II dissolved in a small amt. of satd. NaHCO₃ soln. The mixt. is stirred .apprx.0.5 hr. at 0-5.degree. maintaining the pH at 7-8 by the addn. of NaHCO₃ soln., and the filtered soln. concd. in vacuo, giving 5-methyl-3-(p-guanidinophenyl)-4-isoxazolylicarboxylic acid of the same activity as IV. I is prepd. as follows: 25.3 g. H₂NOH.HCl is added to 50 g. p-O₂NC₆H₄CHO in 500 ml. C₅H₅N, the mixt. is heated .apprx.1 hr. on a steam bath, 3 vols. H₂O added, and the soln. cooled, giving p-O₂NC₆H₄CH:NOH (V), crystd. from EtOH H₂O. V (52 g.) in 202 ml. 8.3N HCl is treated with Cl₂ at 0.degree. for .apprx.1 hr. giving V chloride which (51 g.) in 113 ml. MeOH cooled to 10.degree. is added to a soln. of 18.2 g. NaOMe in 113 ml. MeOH and 44 g. AcCH₂CO₂Et at -25.degree. at such a rate that the temp. is kept below 0.degree.. The mixt. is stirred 18 hrs. at 25.degree., causing the pptn. of the Et ester (VI) of 5-methyl-3-(p-nitrophenyl)-4-isoxazolylicarboxylic acid (VII) which is recrystd. from MeOH-Et₂O. VI (43 g.) is refluxed .apprx.1.5 hrs. in 755 ml. MeOH and 167 ml. N NaOH in a N atm., the cooled soln. neutralized with 20 ml. AcOH and concd. in vacuo, pptg. VII, recrystd. from EtOH. VII (2.4 g.) in 250 ml. MeOH is reduced with H in the presence of 1 g. 5% Rh-C at 40 lb. H pressure to give</p>				

5-methyl-3-(p-aminophenyl)-4-isoxazolylcarboxylic acid (VIII). A soln. of 973 mg. VIII and 362 mg. BzNHCN in 5 ml. EtOH is evapd. on a steam bath to dryness and the residue worked up as above, giving I. Hydrogenolysis of 0.208 g. 6-(p-guanidinophenoxyacetamido)penicillanic acid benzyl ester-HCl (IX) in 10 ml. 50% MeOH in the presence of 0.2 g. Pd-C and countercurrent distribution between BuOH and H₂O give pure p-guanidinophenoxy-methylpenicillin from the aq. soln. IX is prepd. as follows: A mixt. of 1.4 g. p-H₂NC₆H₄OCH₂CO₂H and a soln. of NaOH contg. .apprx.10 meq. NaOH, 2 ml. HCONMe₂, and 1.4 g. S-methylisothionitrourea is stirred 1.5 hrs. at 60.degree., then 10 meq. dil. HCl is added to the cooled mixt., pptg. p-nitroguanidinophenoxyacetic acid (X), m. 239.degree. (decompn.). X (7.3 g.) in 450 ml. 90% aq. MeOH is reduced at 40 lb. H in the presence of 4.5 g. 10% Pd-C to give p-guanidinophenoxyacetic acid-HCl (XI), m. 170.degree.. XI (500 mg.) in 0.87 ml. HCONMe₂ is added to 518 mg. N,N'dicyclohexylcarbodiimide (XII) and 779 mg. II benzyl ester (XIII) in 0.87 ml. HCONMe₂ and the mixt. kept 1 hr. at 25.degree.. It is then centrifuged, the supernatant layer poured off, the ppt. extd. with a 1:1 mixt. of HCONMe₂-CH₂Cl₂ and centrifuged again. The combined solns. are dild. with Et₂O, the pptd. oil is triturated with Et₂O, and the solid material subjected to countercurrent distribution, giving pure IX from the BuOH phase. A mixt. of 153 mg. benzyl 6-(p-guanidinomethylbenzamido)penicillanate-HCl (XIV), 10 mg. NaHCO₃, and 300 mg. 10% Pd-C in 17 ml. 90% aq. MeOH is hydrogenated at atm. pressure .apprx.45 min. The filtered catalyst is washed with MeOH and the combined filtrates are concd. in vacuo to give p-guanidinomethylphenyl penicillin, which inhibits *S. aureus* at 7.8 .gamma./ml. concn. p-NCC₆H₄CO₂H (2 g.) is hydrogenated in 40 ml. EtOH satd. with NH₃ in the presence of 2 g. Raney Ni at 85.degree. and 1500 lb. H pressure. The filtered soln. is acidified with 2.5N HCl, pptg. p-H₂NCH₂C₆H₄CO₂H which (1.2 g.) in 16 ml. H₂O contg. 3.76 ml. concd. NH₄OH and 2.26 g. O-methylisourea-HCl is stirred 18 hrs., and the mixt. dissolved in hot EtOH and repptd. by acidification to pH 2, giving p-guanidinomethylbenzoic acid-HCl. This (374 mg.) in 2 ml. HCONMe₂ is added to a stirred soln. of 500 mg. XII and 1 g. XIII in 2 ml. CH₂Cl₂, the mixt. stirred 0.5 hr. at 25.degree. and 2 hrs. at 0-5.degree., dild. with CH₂Cl₂, and filtered. Addn. of Et₂O to the filtrate ppts. XIV. Treatment of XIII with p-guanidinomethylphenylacetic acid in the presence of XII gives benzyl p-guanidinomethylbenzylpenicillanate-HCl which on hydrogenolysis with Pd-C gives p-guanidinomethylbenzylpenicillin. p-Guanidinophenylacetic acid (XV) (0.2 g.) and 0.3 ml. SOCl₂ 10 min. at 25.degree. give the acid chloride-HCl, m. 127-30.degree. (decompn.), which is treated in 1 ml. tetrahydrofuran and 1 ml. H₂O with 0.23 g. Na salt of II and 2 ml. 0.5N NaHCO₃ 10 min. at 25.degree., giving p-guanidinobenzylpenicillin, m. 195-200.degree. (decompn.); it inhibits *S. aureus* at a concn. of 0.24 .gamma./ml. XV is prepd. by the reaction of 6.04 g. p-H₂NC₆H₄CH₂CO₂H in 15 ml. 2.7N NaOH with 5.4 g. 1-nitro-2-methylisothiurea and catalytic redn. of the p-nitroguanidinophenylacetic acid, m. 188-90.degree., by refluxing it 15 min. with 1 g. Raney Ni in 75 ml. MeOH and hydrogenating the filtered soln. with 1 g. Raney Ni at 40 lb. H pressure 3 hrs. at 25.degree.. In this way 550 mg. XV, m. 320-2.degree. is obtained. 2,6-Dimethoxy-4-guanidinobenzoic acid-HCl (XVI) (274 mg.) in 1 ml. HCONMe₂ is added to 0.31 g. XIII and 0.25 g. XII in 0.5 ml. HCONMe₂, the mixt. is kept 0.5 hr. at 25.degree. the pptd. dicyclohexylurea washed with 2 ml. CH₂Cl₂, and the combined filtrates are dild. with 100 ml. Et₂O, causing the pptn. of PhCH₂ 6- (2,6-dimethoxy-4-guanidinobenzamido)penicillanate-HCl which (300 mg.) is hydrogenated 2 hrs. in 15 ml. 80% aq. MeOH at 40 lb. H in the presence of 10% Pd-C to give 2,6-dimethoxy-4-guanidinophenylpenicillin. XVI is prepd. by refluxing 11 g. 4-bromo-2,6-dimethoxybenzoic acid and 3.7 g. K₂CO₃ 20 hrs. with 6 ml. PhCH₂Br in 100 ml. Me₂CO and evapg. the filtered soln. to give 4,2,6-Br(MeO)₂C₆H₂CO₂CH₂Ph (XVII). XVII (11 g.) is added to a soln. of 1.2 g. Na in 200 ml. liquid NH₃, the soln. stirred 3 hrs., then 3.5 g. NH₄Cl is added and the soln. evapd. The residue is extd. with 150 ml. Et₂O and 100 ml. H₂O, the Et₂O ext. extd. with dil.

H₂SO₄, and the combined aq. solns. are neutralized, giving 4,2,6-H₂N (MeO)₂C₆H₂CO₂CH₂Ph (XVIII), m. 115-16.degree. (MeOH), confirmed by N.M.R. A mixt. of 574 mg. XVIII and 324 mg. BzNHCN in 5 ml. EtOH is evapd. on a steam bath, 5 ml. EtOH added, the soln. heated 1.5 hrs., and the residue heated 45 min. in 5 ml. EtOH with 0.5 ml. 11.7 N NaOH and kept 18 hrs. at 25.degree.. The ppt. formed is dissolved in 20 ml. H₂O, the soln. washed with 20 ml. Et₂O, the aq. soln. acidified to pH 2, washed with Et₂O, concd. to 10 ml., and neutralized with NaHCO₃, giving XVI, m. 220.degree. (decompn.); its HCl salt decomp. at 220.degree. (Me₂CO-Et₂O).

- IT Staphylococcus
(aureus (includes albus and citreus), penicillin deriv. effect on)
- IT Thiazolidinium compounds, 2-[2-[3-(carboxymethyl)-4-oxo-2-thioxo-5-thiazolidinylidene]ethylidene]-3-ethyl-3-methyl-, methyl sulfate
- IT Polyoxymethylenes, polymers, with cellulose triacetate
(reaction with 1,2-benzisothiazolin-3-one derivs.)
- IT 3956-33-0, Acetic acid, (p-guanidinophenyl)- 4085-41-0,
4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[2-(p-guanidinophenyl)acetamido]-3,3-dimethyl-7-oxo- 4255-81-6, Benzoic acid,
4-guanidino-2,6-dimethoxy-, hydrochloride 7035-77-0,
4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[2-(p-guanidinophenoxy)acetamido]-3,3-dimethyl-7-oxo-, benzyl ester,
hydrochloride 7035-78-1, 4-Isloxazolecarboxylic acid,
3-(p-guanidinophenyl)-5-methyl- 7035-79-2, Benzoyl chloride,
p-guanidino-, hydrochloride 7035-80-5, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(p-guanidinobenzamido)-3,3-dimethyl-7-oxo-
7035-81-6, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid,
6-[3-(p-guanidinophenyl)-5-methyl-4-isoxazolecarboxamido]-3,3-dimethyl-7-oxo-
7035-82-7, 4-Isloxazolecarboxylic acid, 5-methyl-3-(p-nitrophenyl)-,
ethyl ester 7035-83-8, 4-Isloxazolecarboxylic acid, 3-(p-aminophenyl)-5-methyl-
7035-84-9, Acetic acid, [p-(3-nitroguanidino)phenoxy]-
7035-85-0, Acetic acid, (p-guanidinophenoxy)-, hydrochloride 7035-86-1,
4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[p-(guanidinomethyl)benzamido]-3,3-dimethyl-7-oxo- 7035-88-3, Acetyl
chloride, (p-guanidinophenyl)-, hydrochloride 7035-90-7, Acetic acid,
[p-(3-nitroguanidino)phenyl]- 7035-91-8, Benzoic acid,
4-amino-2,6-dimethoxy-, benzyl ester 7035-92-9, Benzoic acid,
4-guanidino-2,6-dimethoxy- 7036-09-1, 2,4,5-Thiazolidinetriene,
3-allyl-2-thio- 7036-10-4, 2,4,5-Thiazolidinetriene, 3-dodecyl-2-thio-
7036-11-5, 2,4,5-Thiazolidinetriene, 3-cyclohexyl-2-thio- 7036-12-6,
2,4,5-Thiazolidinetriene, 3-(p-methoxyphenyl)-2-thio- 7123-64-0,
4-Isloxazolecarboxylic acid, 5-methyl-3-(p-nitrophenyl)-
(prepn. of)
- IT 3956-33-0, Acetic acid, (p-guanidinophenyl)-
(prepn. of)
- RN 3956-33-0 HCAPLUS
- CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1965:498281 HCAPLUS

DN 63:98281

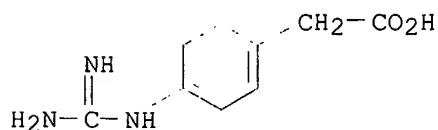
OREF 63:18065b-d

TI Synthesis of guanidino-substituted penicillins and cephalosporins

AU Leanza, W. J.; Christensen, B. G.; Rogers, E. F.; Patchett, A. A.

CS Merch, Sharp & Dohme Res. Labs., Rahway, NJ

- SO Nature (1965), 207(5004), 1395-6
 DT Journal
 LA English
 CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
 AB 6-Benzylaminopenicillanic acid (I) was coupled to D-(-)-.alpha.-guanidinophenylacetic acid by means of dicyclohexyldiimide and the protective benzyl group removed by hydrogenolysis. The resultant 6-D(-)-(.alpha.-guanidinophenylacetamido)penicillanic acid is orally as active as oxacillin against several resistant staphylococcal infections, is stable in acid, and is also highly effective against penicillin sensitive gram-positive infections. If .rho.-guanidinophenylacetyl chloride hydrochloride (II) is coupled with 6-aminopenicillanic acid, 6-(.rho.-guanidinophenylacetamido)penicillanic acid is obtained, and this has 10 times the activity of benzylpenicillin. If 4-guanidino-2,6-dimethoxybenzoyl chloride hydrochloride is coupled with I and hydrogenolyzed, 6-(4-guanidino-2,6dimethoxybenzamido)penicillanic acid is obtained and this is twice as potent as methicillin parenterally in mice against resistant staphylococcal infections. If II is coupled with 7-aminocephalosporanic acid, 7-(.rho.-guanidinophenylacetamido)cephalosporanic acid is obtained, which is more active than methicillin against a resistant staphylococcal infection in mice and is also more active than benzylpenicillin parenterally against penicillin sensitive infections
- IT 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(benzylamino)-3,3-dimethyl-7-oxo-, benzyl ester, hydrochloride
 IT 113-00-8, Guanidine (derivs.)
 IT 1406-05-9, Penicillins 11111-12-9, Cephalosporin (guanidine derivs.)
 IT 1254-56-4, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(benzylamino)-3,3-dimethyl-7-oxo-, benzyl ester 3956-31-8, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-amino-3,3-dimethyl-7-oxo-, benzyl ester 3956-32-9, Acetic acid, [p-(3-benzoylguanidino)phenyl]- 3956-33-0, Acetic acid, (p-guanidinophenyl)- 3956-34-1, Benzoic acid, 4-amino-2,6-dimethoxy-, methyl ester 4003-39-8, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(2-guanidino-2-phenylacetamido)-3,3-dimethyl-7-oxo- 4003-40-1, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-(4-guanidino-2,6-dimethoxybenzamido)-3,3-dimethyl-7-oxo- 4085-40-9, Glycine, N-amidino-2-phenyl-, hydrochloride 4085-41-0, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[2-(p-guanidinophenyl)acetamido]-3,3-dimethyl-7-oxo- 4255-81-6, Benzoic acid, 4-guanidino-2,6-dimethoxy-, hydrochloride 27488-51-3, 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[2-(p-guanidinophenyl)acetamido]-3-(hydroxymethyl)-8-oxo-, acetate (ester) (prepn. of)
 IT 3956-33-0, Acetic acid, (p-guanidinophenyl)- (prepn. of)
 RN 3956-33-0 HCAPLUS
 CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)



=> fil reg

FILE 'REGISTRY' ENTERED AT 15:14:06 ON 14 FEB 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2003 HIGHEST RN 490012-70-9
DICTIONARY FILE UPDATES: 13 FEB 2003 HIGHEST RN 490012-70-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

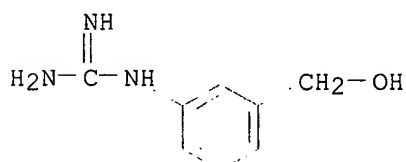
Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d ide can tot

L62 ANSWER 1 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 437384-35-5 REGISTRY
CN Guanidine, [3-(hydroxymethyl)phenyl]-, mononitrate (salt) (9CI) (CA INDEX
NAME)
MF C8 H11 N3 O . H N O3
SR CA
LC STN Files: CA, CAPLUS

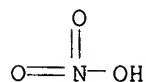
CM 1

CRN 437384-34-4
CMF C8 H11 N3 O



CM 2

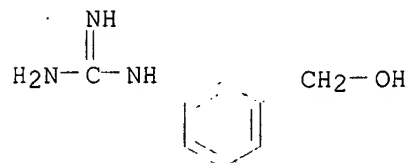
CRN 7697-37-2
CMF H N O3



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

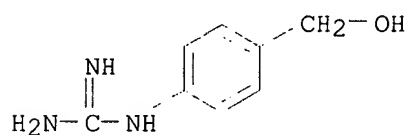
REFERENCE 1: 137:33316

L62 ANSWER 2 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 437384-34-4 REGISTRY
 CN Guanidine, [3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C8 H11 N3 O
 CI COM
 SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L62 ANSWER 3 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 364335-04-6 REGISTRY
 CN Guanidine, [4-(hydroxymethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN N-(4-Hydroxymethylphenyl)guanidine hydrochloride
 MF C8 H11 N3 O . Cl H
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

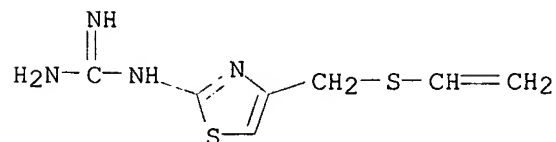


● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

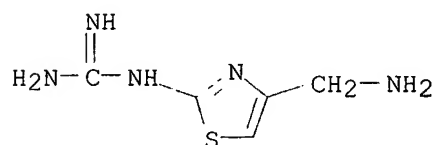
REFERENCE 1: 135:288789

L62 ANSWER 4 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 344302-20-1 REGISTRY
 CN Guanidine, [4-[(ethenylthio)methyl]-2-thiazolyl]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C7 H10 N4 S2
 SR Reaction Database
 LC STN Files: CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L62 ANSWER 5 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 326405-51-0 REGISTRY
CN Guanidine, [4-(aminomethyl)-2-thiazolyl]-, dihydrochloride (9CI) (CA
INDEX NAME)
MF C5 H9 N5 S . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS

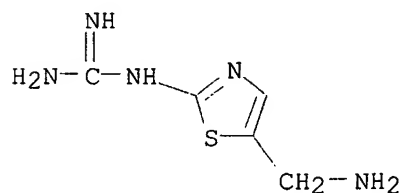


● 2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:178474

L62 ANSWER 6 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 301188-43-2 REGISTRY
CN Guanidine, [5-(aminomethyl)-2-thiazolyl]-, dihydrochloride (9CI) (CA
INDEX NAME)
MF C5 H9 N5 S . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (301188-04-5)



● 2 HCl

3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

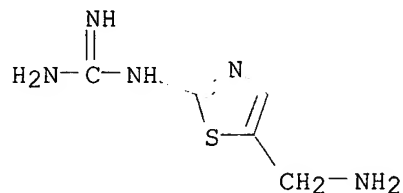
REFERENCE 1: 136:37604

REFERENCE 2: 134:178474

REFERENCE 3: 133:296665

L62 ANSWER 7 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 301188-04-5 REGISTRY
CN Guanidine, [5-(aminomethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C5 H9 N5 S
CI COM
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

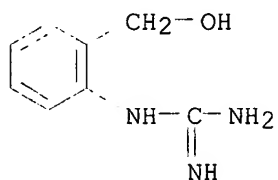
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:296665

L62 ANSWER 8 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 247234-33-9 REGISTRY
CN Guanidine, [2-(hydroxymethyl)phenyl]-, monoacetate (salt) (9CI) (CA INDEX NAME)
MF C8 H11 N3 O . C2 H4 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

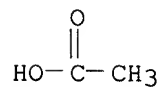
CM 1

CRN 247234-32-8
CMF C8 H11 N3 O



CM 2

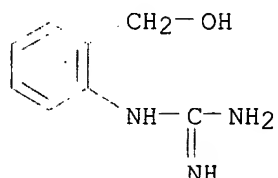
CRN 64-19-7
CMF C2 H4 O2



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

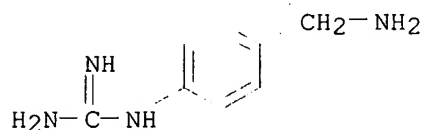
REFERENCE 1: 131:310457

L62 ANSWER 9 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 247234-32-8 REGISTRY
 CN Guanidine, [2-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C8 H11 N3 O
 CI COM
 SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L62 ANSWER 10 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 202979-33-7 REGISTRY
 CN Guanidine, [4-(aminomethyl)phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)
 MF C8 H12 N4 . 2 Cl H
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
 CRN (174959-56-9)



● 2 HCl

4 REFERENCES IN FILE CA (1962 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

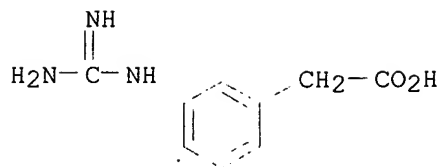
REFERENCE 1: 136:37604

REFERENCE 2: 134:178474

REFERENCE 3: 134:65801

REFERENCE 4: 128:167443

L62 ANSWER 11 OF 42 REGISTRY COPYRIGHT 2003 ACS
 RN 197792-59-9 REGISTRY
 CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, monohydrochloride (9CI)
 (CA INDEX NAME)
 MF C9 H11 N3 O2 . Cl H
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
 CRN (52820-39-0)



● HCl

4 REFERENCES IN FILE CA (1962 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 129:108912

REFERENCE 2: 129:95328

REFERENCE 3: 127:346201

REFERENCE 4: 127:318772

L62 ANSWER 12 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 180146-21-8 REGISTRY

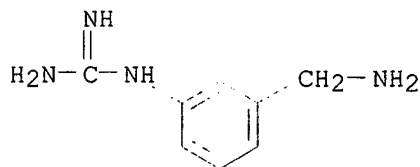
CN Guanidine, [3-(aminomethyl)phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

MF C8 H12 N4 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

CRN (180079-84-9)



● 2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:167546

L62 ANSWER 13 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 180079-84-9 REGISTRY

CN Guanidine, [3-(aminomethyl)phenyl]- (9CI) (CA INDEX NAME)

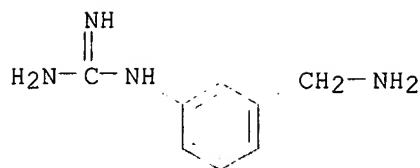
FS 3D CONCORD

MF C8 H12 N4

CI COM

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

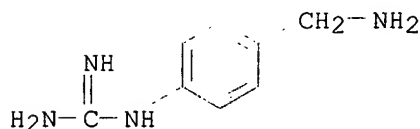
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:167545

L62 ANSWER 14 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 174959-57-0 REGISTRY
CN Guanidine, [4-(aminomethyl)phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)
MF C8 H12 N4 . 2 C2 H F3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

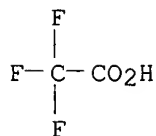
CM 1

CRN 174959-56-9
CMF C8 H12 N4



CM 2

CRN 76-05-1
CMF C2 H F3 O2



4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

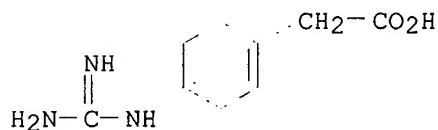
REFERENCE 1: 132:137409

REFERENCE 2: 127:205895

REFERENCE 3: 125:114691

REFERENCE 4: 124:260612

L62 ANSWER 15 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 141029-24-5 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, monohydrochloride (9CI)
(CA INDEX NAME)
MF C9 H11 N3 O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (3956-33-0)

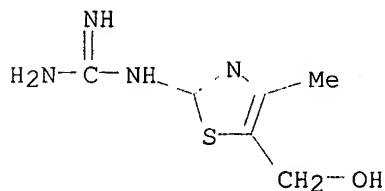


● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 116:214925

L62 ANSWER 16 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 131184-80-0 REGISTRY
CN Guanidine, [5-(hydroxymethyl)-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)
MF C6 H10 N4 O S
SR CA
LC STN Files: CA, CAPLUS

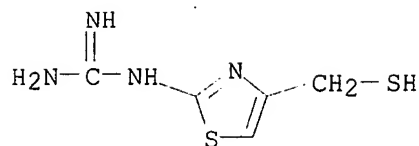


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 114:23844

L62 ANSWER 17 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 130463-38-6 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]-, barium salt (2:1) (9CI) (CA INDEX NAME)
MF C5 H8 N4 S2 . 1/2 Ba
SR CA
LC STN Files: CA, CAPLUS
CRN (95853-51-3)

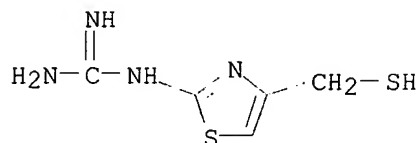


● 1/2 Ba

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 113:231365

L62 ANSWER 18 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 130463-37-5 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]-, calcium salt (2:1) (9CI)
(CA INDEX NAME)
MF C5 H8 N4 S2 . 1/2 Ca
SR CA
LC STN Files: CA, CAPLUS
CRN (95853-51-3)

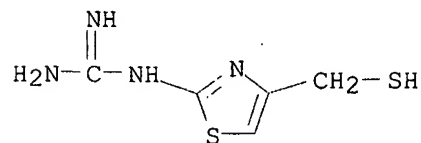


● 1/2 Ca

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 113:231365

L62 ANSWER 19 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 130463-36-4 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]-, monopotassium salt (9CI)
(CA INDEX NAME)
MF C5 H8 N4 S2 . K
SR CA
LC STN Files: CA, CAPLUS
CRN (95853-51-3)

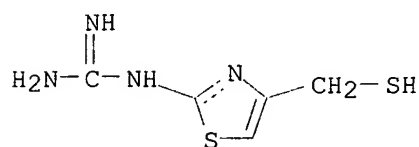


K

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 113:231365

L62 ANSWER 20 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 130463-35-3 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]-, monosodium salt (9CI) (CA INDEX NAME)
MF C5 H8 N4 S2 . Na
SR CA
LC STN Files: CA, CAPLUS
CRN (95853-51-3)

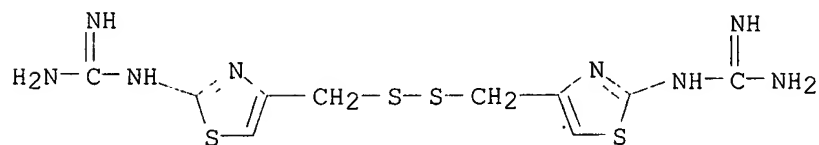


2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:374680

REFERENCE 2: 113:231365

L62 ANSWER 21 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 129083-44-9 REGISTRY
CN Guanidine, N,N''-[dithiobis(methylene-4,2-thiazolediyl)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H14 N8 S4
SR CA
LC STN Files: CA, CAPLUS



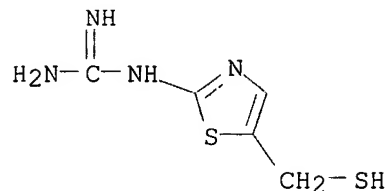
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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 113:178363

L62 ANSWER 22 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 124822-88-4 REGISTRY
CN Guanidine, [5-(mercaptomethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C5 H8 N4 S2
SR CA
LC STN Files: CA, CAPLUS

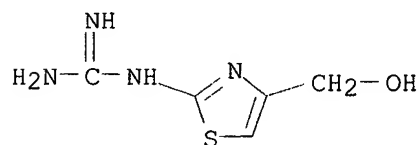


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 112:98516

L62 ANSWER 23 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 119027-63-3 REGISTRY
CN Guanidine, [4-(hydroxymethyl)-2-thiazolyl]-, hydrochloride (9CI) (CA
INDEX NAME)
MF C5 H8 N4 O S . x Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (86794-42-5)

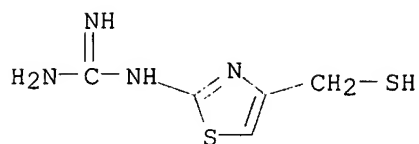


● x HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 110:95220

L62 ANSWER 24 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 102409-46-1 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]-, hydrochloride (9CI) (CA
INDEX NAME)
MF C5 H8 N4 S2 . x Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (95853-51-3)



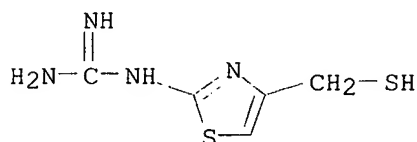
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2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 110:95220

REFERENCE 2: 105:60596

L62 ANSWER 25 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 95853-51-3 REGISTRY
CN Guanidine, [4-(mercaptomethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (2-Guanidinethiazol-4-yl)methyl mercaptan
CN 2-Guanidinethiazole-4-methylthiol
FS 3D CONCORD
MF C5 H8 N4 S2
CI COM
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1962 TO DATE)
7 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 124:261037

REFERENCE 2: 118:109498

REFERENCE 3: 114:122381

REFERENCE 4: 112:77172

REFERENCE 5: 108:131799

REFERENCE 6: 107:236693

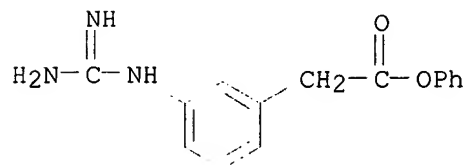
REFERENCE 7: 102:166741

L62 ANSWER 26 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 93131-04-5 REGISTRY
CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, phenyl ester, monomethanesulfonate (9CI) (CA INDEX NAME)
MF C15 H15 N3 O2 . C H4 O3 S

LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

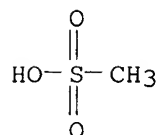
CM 1

CRN 93131-03-4
CMF C15 H15 N3 O2



CM 2

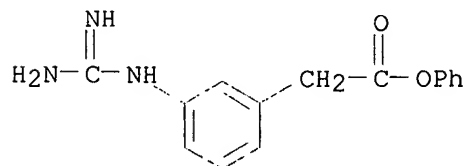
CRN 75-75-2
CMF C H4 O3 S



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 102:5863

L62 ANSWER 27 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 93131-03-4 REGISTRY
CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, phenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H15 N3 O2
CI COM
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

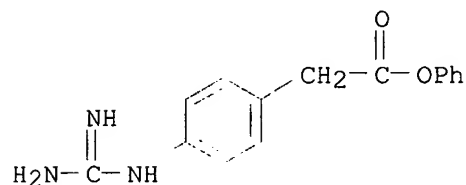
REFERENCE 1: 102:5863

L62 ANSWER 28 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 93130-67-7 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, phenyl ester,
monomethanesulfonate (9CI) (CA INDEX NAME)
MF C15 H15 N3 O2 . C H4 O3 S
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

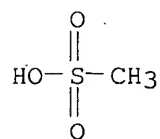
CM 1

CRN 93130-66-6
CMF C15 H15 N3 O2



CM 2

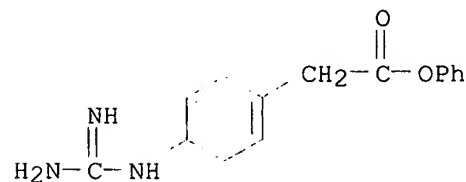
CRN 75-75-2
CMF C H4 O3 S



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 102:5863

L62 ANSWER 29 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 93130-66-6 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, phenyl ester (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C15 H15 N3 O2
CI COM
LC STN Files: CA, CAPLUS

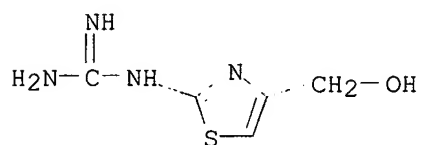


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 102:5863

L62 ANSWER 30 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 86794-42-5 REGISTRY
CN Guanidine, [4-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Guanidino-4-(hydroxymethyl)thiazole
FS 3D CONCORD
MF C5 H8 N4 O S
CI COM
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1962 TO DATE)
6 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 107:77786

REFERENCE 2: 106:67335

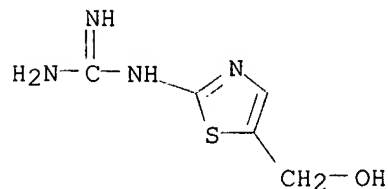
REFERENCE 3: 106:67294

REFERENCE 4: 106:18537

REFERENCE 5: 102:149259

REFERENCE 6: 99:88191

L62 ANSWER 31 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 78441-93-7 REGISTRY
CN Guanidine, [5-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C5 H8 N4 O S
LC STN Files: CA, CAPLUS, USPATFULL

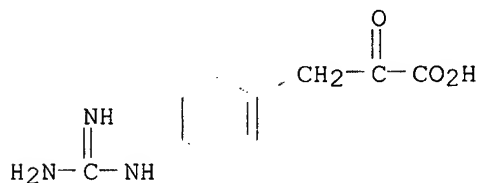


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1962 TO DATE)
8 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 114:228922
REFERENCE 2: 114:23844
REFERENCE 3: 111:153813
REFERENCE 4: 102:78888
REFERENCE 5: 101:7163
REFERENCE 6: 99:194974
REFERENCE 7: 99:139947
REFERENCE 8: 95:62220

L62 ANSWER 32 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 54050-85-0 REGISTRY
CN Benzenepropanoic acid, 4-[(aminoiminomethyl)amino]-.alpha.-oxo- (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C10 H11 N3 O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

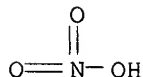
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 82:40064

L62 ANSWER 33 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 52841-31-3 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, mononitrate (9CI) (CA
INDEX NAME)
MF C9 H11 N3 O2 . H N O3
LC STN Files: CA, CAPLUS

CM 1

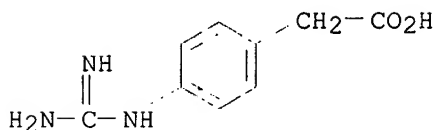
CRN 7697-37-2
CMF H N O3



CM 2

CRN 3956-33-0

CMF C9 H11 N3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:49380

L62 ANSWER 34 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 52820-41-4 REGISTRY

CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

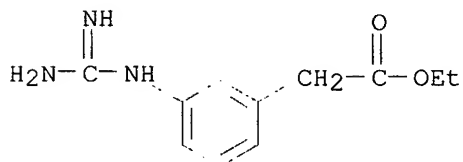
FS 3D CONCORD

MF C11 H15 N3 O2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:165375

L62 ANSWER 35 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 52820-39-0 REGISTRY

CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)

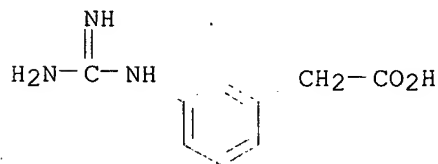
FS 3D CONCORD

MF C9 H11 N3 O2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

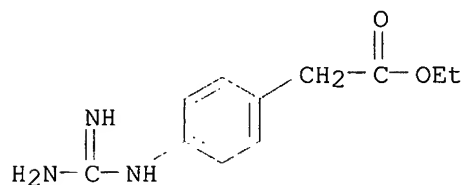
REFERENCE 1: 81:165375

REFERENCE 2: 81:49380

L62 ANSWER 36 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 52779-36-9 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, ethyl ester, mononitrate
(9CI) (CA INDEX NAME)
MF C11 H15 N3 O2 . H N O3
LC STN Files: CA, CAPLUS

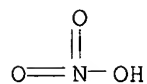
CM 1

CRN 15676-15-0
CMF C11 H15 N3 O2



CM 2

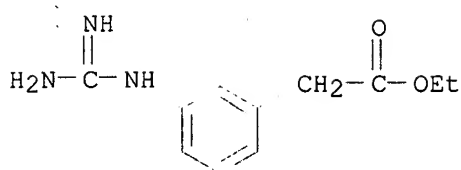
CRN 7697-37-2
CMF H N O3



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:49380

L62 ANSWER 37 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 52779-35-8 REGISTRY
CN Benzeneacetic acid, 3-[(aminoiminomethyl)amino]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF C11 H15 N3 O2 . Cl H
LC STN Files: CA, CAPLUS
CRN (52820-41-4)

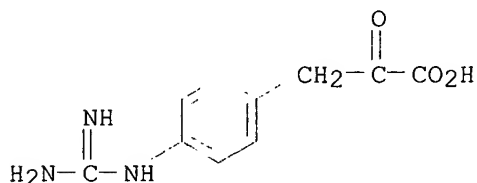


● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:49380

L62 ANSWER 38 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 52779-31-4 REGISTRY
CN Benzenepropanoic acid, 4-[(aminoiminomethyl)amino]-.alpha.-oxo-,
monohydrochloride (9CI) (CA INDEX NAME)
MF C10 H11 N3 O3 . Cl H
LC STN Files: CA, CAPLUS
CRN (54050-85-0)



● HCl

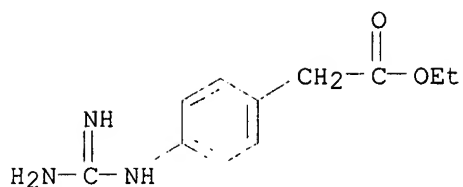
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:49380

L62 ANSWER 39 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 18219-43-7 REGISTRY
CN Acetic acid, (p-guanidinophenyl)-, ethyl ester, monopicrate (8CI) (CA
INDEX NAME)
OTHER NAMES:
CN Ethyl p-guanidinophenylacetate monopicrate
MF C11 H15 N3 O2 . C6 H3 N3 O7
LC STN Files: CA, CAPLUS

CM 1

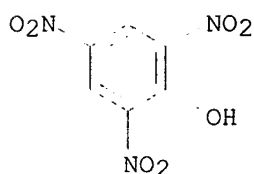
CRN 15676-15-0
CMF C11 H15 N3 O2



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 68:19025

L62 ANSWER 40 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 18219-40-4 REGISTRY

CN Acetic acid, (p-guanidinophenyl)-, ethyl ester, monohydrochloride (8CI)
(CA INDEX NAME)

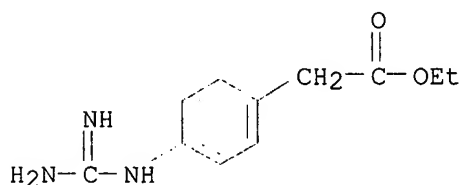
OTHER NAMES:

CN Ethyl p-guanidinophenylacetate monohydrochloride

MF C11 H15 N3 O2 . Cl H

LC STN Files: CA, CAPLUS

CRN (15676-15-0)



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

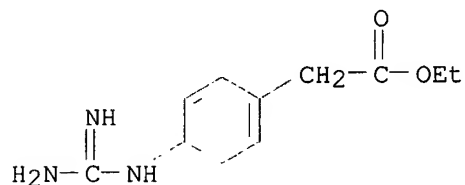
REFERENCE 1: 68:19025

L62 ANSWER 41 OF 42 REGISTRY COPYRIGHT 2003 ACS

RN 15676-15-0 REGISTRY

CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]-, ethyl ester (9CI) (CA
INDEX NAME)

FS 3D CONCORD
MF C11 H15 N3 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

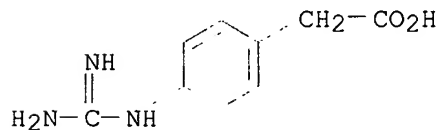


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 81:165375

L62 ANSWER 42 OF 42 REGISTRY COPYRIGHT 2003 ACS
RN 3956-33-0 REGISTRY
CN Benzeneacetic acid, 4-[(aminoiminomethyl)amino]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetic acid, (p-guanidinophenyl)- (7CI, 8CI)
OTHER NAMES:
CN (p-Guanidinophenyl)acetic acid
FS 3D CONCORD
MF C9 H11 N3 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, IFICDB, IFIPAT, IFIUDB,
TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1962 TO DATE)
9 REFERENCES IN FILE CAPLUS (1962 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 124:185543

REFERENCE 2: 84:44102

REFERENCE 3: 81:165375

REFERENCE 4: 78:147591

REFERENCE 5: 72:43668

REFERENCE 6: 67:21905
REFERENCE 7: 66:115703
REFERENCE 8: 65:47730
REFERENCE 9: 63:98281